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The crystal structure of sodium xanthate dihydrate

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Cristallografia. — *The crystal structure of sodium xanthate dihydrate* (*). Nota di FIORENZO MAZZI, VITTORIO TAZZOLI e LUCIANO UNGARETTI, presentata (**) dal Socio G. CAROBBI.

RIASSUNTO. — Lo xantogenato di sodio biidrato ha formula chimica: $C_2H_5COS_2Na \cdot 2H_2O$; quattro unità stechiometriche sono contenute nella cella elementare. Il gruppo spaziale è $P\bar{1}$; le costanti reticolari sono le seguenti: $a = 11.59$, $b = 12.56$, $c = 6.68$ Å, $\alpha = 95°5'$, $\beta = 115°\,18'$, $\gamma = 100°\,25'$. Per la determinazione della struttura cristallina sono state riprese mediante fotogrammi di Weissemberg 3152 riflessioni con le quali sono state effettuate sintesi di Patterson tridimensionali; data la difficoltà di interpretazione delle stesse, dovuta alla non eccessiva differenza in numero atomico degli atomi presenti e alle numerose soprapposizioni derivanti da una spiccata pseudosimmetria, la struttura è stata risolta mediante la applicazione dei metodi diretti. Il raffinamento è stato eseguito col metodo dei minimi quadrati applicando alla fine fattori termici anisotropi per tutti gli atomi. Il fattore di discordanza per i riflessi osservati (2105) dopo nove cicli è 0.071.

Dei due radicali xantogenici indipendenti presenti nella cella elementare uno è perfettamente planare, mentre nell'altro il carbonio del gruppo metilico si discosta dal piano individuato dagli altri atomi formando con esso un angolo di 70° 24'. Gli atomi di sodio coordinano quattro atomi di ossigeno e due atomi di solfo di due diversi gruppi xantogenici formando ottaedri distorti collegati fra loro attraverso spigoli a formare strati paralleli a (010).

INTRODUCTION.

Sodium xanthate can be prepared by reaction among ethanol, sodium hydroxide and carbon disulfide either in aqueous or ethanolic solution according to the equation:

$$C_2H_5OH + NaOH + CS_2 + H_2O \rightarrow NaS_2COC_2H_5 \cdot 2H_2O\ ,$$

followed by slow evaporation of the solution or cooling.

The crystals prepared in this way show in their stoichiometric unit two water molecules, according to the chemical analysis confirmed by the determination of the crystal structure. X ray powder diffrattograms have been carried out on crystals prepared under several different conditions; in any case one obtains identical results corresponding to the data listed in the ASTM card, on which however a formula unit without water molecules is reported. The same results are given by the commercial sodium xanthate, which has to be therefore considered dihydrate.

The crystals heated at 70° C lose a weight corresponding to the water molecules and the diffrattogram carried out just after the heating is somewhat different from that of the dihydrate compound. However the heated xanthate, if exposed to the air, increases in weight and the diffrattogram of this material is again identical to that of the dihydrate compound. One may suggest that

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(*) This work was performed in the Sezione di Pavia del Centro Nazionale di Cristallografia del C.N.R., Istituto di Mineralogia dell'Università.

(**) Nella seduta dell'8 marzo 1969.

the two water molecules lost in the heating, are soon resumed during the exposition to the air. The examination of the differential thermal analysis diagrams leads to the same conclusion: an endothermal peak at 70° C is present for both the dihydrate xanthate and the heated xanthate exposed to the air, whereas it is absent in the just heated xanthate.

The crystals of sodium xanthate dihydrate are pale yellow in color, triclinic pinacoidal, needlelike and elongated following a direction assumed as *c* axis. They show a perfect cleavage parallel to the pinacoid assumed as {010}.

The unit cell parameters are as follows:

$$a = 11.59 \pm 0.02 \text{ Å} \qquad \alpha = 95^\circ\, 5' \pm 10'$$
$$b = 12.56 \pm 0.02 \text{ Å} \qquad \beta = 115^\circ\, 18' \pm 10'$$
$$c = 6.68 \pm 0.02 \text{ Å} \qquad \gamma = 100^\circ\, 25' \pm 10'$$
$$\text{space group } P\bar{1} \quad , \quad Z = 4 \quad , \quad D_x = 1.408$$

EXPERIMENTAL.

For the collection of the experimental data, the crystal was rotated about the *c* axis and Weissemberg equi-inclination integrated photographs were obtained for reciprocal lattice levels from $l = 0$ to $l = 5$ using nickel filtered copper radiation and the multiple-film technique. A total of 3152 reflexions, out of about 3800 present in the CuKα limiting sphere (82 %) were inspected; 2105 of them were measured photometrically, the remaining 1047 were either too faint to be suitably measured or did not give any blackening on the films. The intesities were corrected for the Lorentz-polarization factor and for α_1—α_2 splitting effect, taking into account the integration technique which complicates the splitting effect for its diagonal direction with respect to the sides of the film. No correction for the absorption was made because of the small cross-section of the crystal and its low absorption coefficient.

The intensities for the different levels were put approximately on the absolute scale by the Wilson method; the scale factors for each level were successively improved during the least squares refinement before the application of an anisotropical thermal factor to the atoms.

CRYSTAL STRUCTURE ANALYSIS.

As the N(z) test for the presence of the inversion center was positive, the resolution of the crystal structure was attempted in the space group $P\bar{1}$; furthermore an examination of the observed values of the structure amplitudes (*Fo*'s with *h* even generally higher than those with *h* odd) showed the presence of a pseudo-cell with a halved *a*-period.

The study of a three-dimensional Patterson synthesis obtained from the experimental data did not allow to reach any clear conclusion about the atomic parameters, very likely because of the small differences in the atomic number of most of the atoms and for the presence of superimpositions of interatomic vectors.

Then the application of direct methods was tried for the determination of the phases of the structure factors: for this purpose 255 strong reflections (all with h even) were chosen and the Sayre [1] relation:

$$S(hkl) = S(h'k'l')\, S(h+h', k+k', l+l')$$

was used for the determination of their signs.

Owing to the rather high value of the unitary structure amplitudes of these reflections, there was a strong probability for a correct identification of their phases. In this way, by using the Woolfson [2] procedure, together with a set of invariant reflections with surely positive signs, two more groups were derived, each of them including reflections of probably equal sign. By assigning alternatively to the last two sets of reflections either positive or negative signs, two-dimensional ($hk0$) Fourier syntheses were prepared and one of them allowed the determination of plausible x– and y–parameters for sulfur, sodium and some oxygen atoms: the interpretation of these Fourier projections was obviously complicated by the use of the sole structure factors with h even, so that they showed superimposed the positions of the atoms belonging to the two pseudocells with period $a/2$, in which the true unit cell is split. Once known two of the positional parameters of some atoms, it was possible to recognize their interatomic vectors in the Patterson synthesis, so as to derive from it also the third parameter. Finally a three-dimensional Fourier synthesis, obtained by using the preceding data as starting point, led to the determination of the parameters of the remaining atoms with the obvious exclusion of hydrogens.

Four cycles of least squares refinement with individual isotropic thermal factors carried out on the observed reflexions, using the ORFLS program by Busing, Martin and Levy, lowered the discrepancy factor from $R = 0.22$ to $R = 0.148$. At this stage, after an inspection of a threedimensional difference synthesis, it was decided to continue the least squares refinement with anisotropical thermal factors for the atoms. Four more cycles further lowered the discrepancy factor to $R = 0.073$ for the observed reflections ($R = 0.109$ for all the reflections). On another three-dimensional difference synthesis it was then possible to derive the parameters of the 18 hydrogen atoms in the unit cell (Table VI) which, in the limits of the obtained accuracy, form with the adjacent carbon or oxygen atoms bond lengths and angles comparable with those reported in the literature (Table VII). A final calculation of the the structure factors, following the introduction of the hydrogen parameters gave an R–factor equal to 0.071 for all the observed reflections.

The structure factors were calculated by using the HFS scattering factors for neutral atoms published by Hanson, Herman, Lea and Skillmann [3].

The observed and calculated structure factors are compared in Table I. Positional parameters are listed in Table II and anisotropical thermal factors in Table III; the analysis of the latter is shown in Table IV; bond lengths and angles are summarized in Table V.

TABLE I.

Observed (F_o) *and calculated* (F_c) *structure factors.*

Reflections marked with an asterisk were unobservably weak; in this case F_o derives from $0.5\ I_{min}$.

h	*k*	*l*	F_o	F_c
0	0	2	14.2	15.0
0	0	3	62.4	66.8
0	0	4	28.6	-28.2
0	0	5	9.8	-6.9
0	1	1	46.3	-44.5
0	1	2	40.1	36.9
0	-1	2	12.1	9.1
0	1	3	26.1	24.4
0	-1	3	55.0	61.5
0	1	4	13.7	-12.0
0	-1	4	4.5	-2.3
0	1	5	18.7	-16.9
0	-1	5	13.9	14.2
0	2	0	18.8	-15.9
0	2	1	33.2	-30.9
0	-2	1	43.0	-38.6
0	2	2	76.8	-74.7
0	-2	2	51.8	50.1
0	2	3	21.4	-17.9
0	-2	3	70.1	77.9
0	2	4	5.5	-6.1
0	-2	4	14.9	15.6
0	2	5	29.8	-30.6
0	-2	5	26.0	25.0
0	3	0	42.0	43.2
0	3	1	6.6	5.4
0	-3	1	19.0	-18.4
0	3	2	60.2	-60.4
0	-3	2	7.9	-6.8
0	3	3	16.8	-17.6
0	-3	3	40.0	39.7
0	3	4	26.1	-26.5
0	-3	4	23.2	-21.3
0	3	5	24.8	-25.1
0	-3	5	17.6	18.7
0	4	0	59.3	-66.6
0	4	1	19.7	-18.3
0	-4	1	14.2	-13.2
0	4	2	6.0	-5.0
0	-4	2	61.7	-66.6
0	4	3	11.4	-9.8
0	-4	3	7.2	-4.5
0	4	4	8.8	-8.3
0	-4	4	6.7	-6.0
0	4	5	11.7	-9.7
0	-4	5*	2.1	3.4
0	5	0	61.9	-66.9
0	5	1	29.9	-26.6
0	-5	1	19.8	-18.1
0	5	2	48.5	-46.7
0	-5	2	17.0	-14.3
0	5	3*	2.3	-1.8
0	-5	3	13.6	-11.4
0	5	4	11.7	11.2
0	-5	4*	2.2	.7
0	5	5*	2.7	-1.1
0	-5	5	18.1	-16.1
0	6	0	13.0	-9.1
0	6	1	11.8	-11.1
0	-6	1	46.4	-47.0
0	6	2	26.1	-24.8
0	-6	2	13.2	-11.4
0	6	3	20.8	19.6
0	-6	3	28.4	-27.8
0	6	4	6.5	-7.4
0	-6	4	30.1	-32.6
0	6	5	13.4	12.5
0	-6	5	16.8	-17.1
0	7	0	47.5	47.2
0	7	1	5.6	5.0
0	-7	1	31.1	-31.0
0	7	2	29.5	28.2
0	-7	2	46.9	-45.4
0	7	3	36.3	38.7
0	-7	3	4.2	-3.0
0	7	4	7.9	7.3
0	-7	4	11.9	-11.8
0	7	5	15.1	16.4
0	-7	5	16.9	-17.7
0	8	0	35.8	35.7
0	8	1	14.8	13.1
0	-8	1	15.4	15.0
0	8	2	20.9	20.5
0	-8	2	15.4	15.2
0	8	3	27.3	28.7
0	-8	3	5.8	4.6
0	8	4	16.5	18.2
0	-8	4	8.0	-7.6
0	8	5*	2.6	4.5
0	-8	5	17.7	-17.8
0	9	0	43.5	44.1
0	9	1	16.6	16.0
0	-9	1*	3.4	2.7
0	9	2*	3.0	-3.5
0	-9	2	38.4	37.1
0	9	3	10.3	10.1
0	-9	3	18.4	15.5
0	9	4	6.6	-6.6
0	-9	4	15.3	-15.2
0	9	5	4.4	-5.6
0	-9	5*	2.8	4.2
0	10	0	35.5	37.8
0	10	1*	3.7	.6
0	-10	1*	3.6	-3.2
0	10	2	5.9	5.4
0	-10	2*	2.9	1.4
0	10	3*	2.8	.9
0	-10	3	39.8	40.5
0	10	4	7.9	-8.6
0	-10	4	7.1	7.4
0	10	5	4.4	-4.4
0	-10	5	16.0	16.8
0	11	0	10.9	-11.1
0	11	1	7.5	-7.6
0	-11	1	15.2	14.2
0	11	2*	3.0	-1.6
0	-11	2	10.3	10.4
0	11	3	9.0	-10.0
0	-11	3	18.0	18.2
0	11	4*	2.5	2.2
0	-11	4	12.0	12.1
0	-11	5	8.8	8.7
0	12	0*	4.9	-4.7
0	12	1*	3.6	1.2
0	-12	1*	3.8	-1.0
0	12	2	16.9	-18.8
0	-12	2	8.6	7.1
0	12	3	9.2	-10.0
0	-12	3*	2.9	-.7
0	-12	4*	3.1	-3.5
0	-12	5	6.4	5.7
0	13	0	8.5	-7.8
0	13	1	10.3	-11.1
0	-13	1	15.2	-14.6
0	13	2	7.8	-8.1
0	-13	2	13.8	-15.1
0	13	3	5.5	-5.4
0	-13	3*	2.7	-.1
0	-13	4*	3.1	-1.7
0	-13	5	6.9	7.2
0	14	0	20.5	-22.3
0	14	1	11.5	-14.3
0	-14	1	7.6	-6.5
0	14	2	5.3	-5.2
0	-14	2	10.0	-10.2
0	-14	3*	2.5	-2.7
0	-14	4	4.7	4.4
0	15	0*	3.5	-1.8
0	15	1*	1.9	4.2
0	-15	1	5.0	-4.0
0	15	2*	5.3	-3.1
0	-15	2*	2.3	-3.5
0	-15	3	13.2	-15.2
0	16	1*	1.8	4.5
1	0	0*	.0	4.4
1	0	1	18.8	-17.1
1	0	2	4.6	1.8
1	0	3	6.0	-7.1
1	0	-3	40.1	47.2
1	0	4	7.3	-7.1
1	0	-4	17.3	-17.6
1	0	5	10.9	9.6
1	0	-5	20.4	-20.8
1	-1	0*	.0	-4.2
1	1	1	33.1	29.5
1	-1	1	27.0	-24.1
-1	1	1	5.6	-7.4
1	1	2	28.2	-25.8
1	-1	2	14.0	-11.1
-1	1	2	6.0	5.1
1	1	3	15.1	-14.9
1	1	-3	12.6	-15.5
1	-1	3	11.8	13.0
-1	1	3	10.3	-12.0
1	1	4	11.4	10.8
1	1	-4	2.4	2.0
1	-1	4	29.7	-29.7
-1	1	4	12.6	-12.9
1	1	5*	2.5	2.0
1	1	-5	7.8	-6.1
1	-1	5	21.1	-21.2
-1	1	5	17.9	18.0
1	2	0*	1.9	1.2
1	-2	0	6.6	4.6
1	2	1	7.2	-5.5
1	2	-1	11.6	-11.3
1	-2	1	50.9	53.0
-1	2	1	23.1	-20.7
1	2	2	15.2	-15.1
1	2	-2	25.6	23.0
1	-2	2	32.0	-32.3
-1	2	2	7.9	-7.3
1	2	3	27.5	28.2
1	2	-3	7.6	8.9
1	-2	3	23.1	-22.4
-1	2	3	36.8	-37.1
1	2	4*	2.5	.0
1	2	-4	18.2	20.6
1	-2	4*	2.1	.4
-1	2	4*	1.9	-.6
1	2	5	6.1	-5.3
1	2	-5	35.2	38.5
1	-2	5	23.1	-22.4
-1	2	5	7.6	-6.4
1	3	0*	2.3	-1.3
1	-3	0	16.6	-13.7
1	3	1	10.0	-6.6
1	3	-1	29.4	-27.9
1	-3	1	32.9	-29.2
-1	3	1	42.1	39.6
1	3	2	6.4	5.3
1	3	-2	31.5	32.1
1	-3	2	31.8	30.1
-1	3	2	4.5	-1.7
1	3	3*	2.1	1.6
1	3	-3	42.5	41.6
1	-3	3	5.3	-6.4
-1	3	3	8.2	7.2
1	3	4	5.3	4.8
1	3	-4*	1.6	1.3
1	-3	4	13.0	11.4
-1	3	4	6.3	6.9
1	3	5	11.9	11.1
1	3	-5	4.2	3.8
1	-3	5	10.1	8.3
-1	3	5	19.0	-18.6
1	4	0*	2.7	-2.1
1	-4	0	12.4	10.4
1	4	1	26.3	27.2
1	4	-1	33.8	31.7
1	-4	1	3.5	1.1
-1	4	1	38.9	-37.5
1	4	2	4.2	3.3
1	4	-2	4.8	-5.4
1	-4	2	28.6	29.2
-1	4	2	6.3	-5.8
1	4	3	16.8	-17.3
1	4	-3	38.2	-35.5
1	-4	3	18.7	19.0
-1	4	3*	1.9	.5
1	4	4	16.2	16.0
1	4	-4	4.0	3.0
1	-4	4*	2.2	-1.5
-1	4	4	6.1	-6.8
1	4	5*	2.7	1.3
1	4	-5	12.2	-11.3
1	-4	5	5.0	3.7
-1	4	5	4.9	3.8
1	5	0	10.4	-10.2
1	-5	0	9.6	8.3
1	5	1	27.0	25.3
1	5	-1	47.3	-47.9
1	-5	1	23.7	22.0
-1	5	1	29.2	29.0
1	5	2	11.7	-11.9
1	5	-2	5.7	7.3
1	-5	2	8.6	7.4
-1	5	2	10.5	7.7
1	5	3	14.8	14.4
1	5	-3	23.8	-21.5
1	-5	3	5.9	-5.7
-1	5	3	29.8	-28.7
1	5	4	14.3	16.6
1	5	-4*	2.0	4.2
1	-5	4*	2.4	1.7
-1	5	4	10.2	9.8
1	5	5	8.1	-7.6
1	5	-5	17.8	17.4
1	-5	5*	2.7	-2.8
-1	5	5*	2.7	2.9
1	6	0	5.7	-4.2
1	-6	0	25.1	-22.9
1	6	1	25.2	-27.5
1	6	-1	19.1	-17.8
1	-6	1	37.5	-37.8
-1	6	1	41.3	41.9
1	6	2	4.8	-4.6
1	6	-2	10.0	9.8
1	-6	2	19.3	18.2
-1	6	2	19.7	-18.9
1	6	3	7.1	7.1
1	6	-3	21.4	18.4
1	-6	3	15.7	-13.9
-1	6	3	6.0	5.7
1	6	4*	3.0	-3.0
1	6	-4	10.2	-10.0
1	-6	4	13.4	14.1
-1	6	4	25.7	27.0
1	6	5*	2.6	-2.0
1	6	-5	5.2	5.2
1	-6	5	26.6	27.5
-1	6	5	6.9	-5.5
1	7	0	7.0	6.9
1	-7	0	11.0	-10.8
1	7	1	15.7	15.1
1	7	-1	21.6	20.3
1	-7	1*	2.7	2.5
-1	7	1	22.6	-21.0
1	7	2*	2.8	2.5
1	7	-2	3.4	-4.4
1	-7	2	36.9	35.3
-1	7	2	19.2	-18.5
1	7	3	14.7	-14.8
1	7	-3	14.3	-13.1
1	-7	3	19.3	18.8
-1	7	3	13.4	12.4
1	7	4*	3.0	-3.0
1	7	-4	22.7	-23.4
1	-7	4	8.0	7.6
-1	7	4*	3.0	3.5
1	7	5	7.2	-7.8
1	7	-5	17.7	-18.7
1	-7	5	23.0	24.3
-1	7	5*	2.8	3.2
1	8	0*	4.2	3.7
1	-8	0	12.5	-11.7
1	8	1	28.9	30.0
1	8	-1	40.1	-41.5
1	-8	1	11.1	7.8
-1	8	1	28.1	29.4
1	8	2	14.2	-14.2
1	8	-2	9.6	-8.2
1	-8	2*	2.5	2.3
-1	8	2	16.3	17.8
1	8	3	6.6	7.4
1	8	-3	19.9	-19.1
1	-8	3	13.4	-13.7
-1	8	3	19.5	-20.1
1	8	4	5.6	4.8
1	8	-4	22.0	-23.6
1	-8	4	13.4	-11.9
-1	8	4*	3.1	2.7
1	8	5	9.2	-9.6
1	8	-5*	2.6	1.3
1	-8	5*	2.7	-1.2
-1	8	5*	2.7	4.6
1	9	0	8.0	8.8
1	-9	0	31.1	-31.3
1	9	1	16.9	-16.5
1	9	-1	11.0	-9.2
1	-9	1	22.7	-20.6
-1	9	1	23.2	23.4
1	9	2	15.8	-18.4
1	9	-2	18.1	18.0
1	-9	2	21.7	-21.5
-1	9	2*	2.9	-1.6
1	9	3	9.3	10.0
1	9	-3	22.0	21.3
1	-9	3	39.5	-40.2
-1	9	3*	2.9	-5.3
1	9	4	5.2	-4.1
1	9	-4	7.8	-8.1
1	-9	4*	3.0	-1.2
-1	9	4	12.9	12.8
1	9	5*	1.9	-.0
1	9	-5	10.6	9.5
1	-9	5*	2.9	2.5
-1	9	5	5.6	-5.3
1	10	0	9.2	8.5
1	-10	0	10.9	-10.8
1	10	1	10.8	10.7
1	10	-1	18.1	16.0
1	-10	1*	3.6	1.2
-1	10	1	13.3	-12.5
1	10	2*	3.0	-.3
1	10	-2	24.3	24.4
1	-10	2	15.0	14.5
-1	10	2	10.2	-10.0
1	10	3	8.3	-8.4
1	10	-3	14.5	14.3
1	-10	3*	2.8	-.9
-1	10	3*	2.8	2.6
1	10	4*	2.7	.1
1	10	-4	7.8	-6.4
1	-10	4*	3.1	-3.3
-1	10	4*	3.1	-1.8
1	10	-5*	2.8	-.9
1	-10	5*	2.8	-4.4
-1	10	5*	2.1	1.3
1	11	0*	4.9	-5.1
1	-11	0*	4.9	5.3
1	11	1	20.9	23.6
1	11	-1	16.6	-16.9
1	-11	1	21.2	19.9
-1	11	1*	3.8	4.8
1	11	2*	2.9	-4.1
1	11	-2*	3.0	5.4
1	-11	2*	3.0	2.8
-1	11	2	13.0	14.5
1	11	3*	2.6	.4
1	11	-3	11.0	-10.5
1	-11	3	8.0	-7.7
-1	11	3	11.6	-12.3
1	11	4	6.2	7.6
1	11	-4*	3.2	6.3
1	-11	4	11.4	-11.4
-1	11	4	4.7	-4.5
1	11	-5	14.5	16.2
1	-11	5	12.5	-14.4
-1	11	5*	1.4	3.0
1	12	0*	4.8	-3.1
1	-12	0	9.1	-9.2
1	12	1*	4.5	-4.6
1	12	-1	10.8	-9.9
1	-12	1*	3.8	-1.2
-1	12	1	12.0	12.7
1	12	2	7.5	-9.3
1	12	-2	14.5	14.3
1	-12	2	8.3	-8.6
-1	12	2	7.5	7.2
1	12	3*	2.2	3.8
1	12	-3	7.7	7.3
1	-12	3	14.5	-13.3
-1	12	3	4.6	-4.7
1	12	-4	7.6	7.0
1	-12	4	7.4	6.6
-1	12	4	5.1	5.3
1	12	-5	13.0	14.2
1	-12	5*	2.5	-1.5
1	13	0*	4.7	-.1
1	-13	0*	4.7	-1.6
1	13	1*	3.5	-.8
1	13	-1	10.2	9.2
1	-13	1*	3.3	-4.7
-1	13	1*	3.4	.3
1	13	2*	2.5	1.6
1	13	-2	7.8	8.1
1	-13	2	15.7	17.3
-1	13	2	7.5	-7.9
1	13	3*	1.4	-6.2
1	13	-3*	2.7	1.9
1	-13	3	6.2	6.6
-1	13	3*	2.2	2.3
1	13	-4*	3.1	-2.7
1	-13	4*	3.0	3.7
1	13	-5*	2.4	-.6
1	-13	5	5.1	5.4
1	14	0	8.8	-9.4
1	-14	0	9.9	10.3
1	14	1	6.6	7.8
1	14	-1	5.4	-4.7
1	-14	1	14.1	13.4
-1	14	1*	3.0	-1.9
1	14	2*	1.7	1.6
1	14	-2	4.2	-4.5
1	-14	2	8.7	9.3
-1	14	2*	2.4	-.1
1	14	-3	10.0	-11.6
1	-14	3	3.9	4.2
1	14	-4	4.5	5.4
1	-14	4*	2.4	-.2
1	15	0*	3.2	-4.3
1	-15	0	6.6	-7.2
1	15	1*	1.9	-.9
1	15	-1	11.9	-12.7
1	-15	1*	2.7	2.0
-1	15	1	7.5	8.8
1	15	-2*	2.1	.5
1	-15	2	3.5	4.4
-1	15	2*	1.3	4.2
1	15	-3*	2.1	-1.1
1	-15	3*	2.3	.4
1	-16	1	7.2	-8.9
2	0	0	27.5	-29.8
2	0	1	71.7	-79.4
2	0	-1	19.9	18.6
2	0	2	18.3	18.3
2	0	3	21.6	-20.6
2	0	4	27.2	-25.5
2	0	5	4.7	-3.9
2	0	-5	2.3	3.3
2	1	0	100.5	-113.0
2	-1	0	84.4	93.1
2	1	1	104.5	-119.3
2	1	-1	79.7	-84.2
2	-1	1	10.6	-11.4
-2	1	1	61.1	64.9
2	1	2	18.3	-18.2
2	-1	2	10.8	-13.2
-2	1	2	47.4	45.9
2	1	3	22.0	-21.9
2	-1	3	22.0	-21.0
-2	1	3	31.2	32.8
2	1	4	19.0	-17.7
2	-1	4	50.2	-52.8
-2	1	4	28.6	31.6
2	1	5	9.0	7.1
2	1	-5*	1.0	-.3
2	-1	5	8.2	-7.1
-2	1	5	3.8	4.2
2	2	0	70.5	73.9
2	-2	0	16.8	14.4
2	2	1	84.9	-92.9
2	2	-1	11.5	-10.0
2	-2	1	39.4	38.4
-2	2	1	7.6	4.9
2	2	2	17.1	15.3
2	2	-2	111.9	-127.3
2	-2	2	37.4	-32.0
-2	2	2	85.7	88.4
2	2	3	4.9	-2.4
2	2	-3	14.3	20.1
2	-2	3	17.1	14.5
-2	2	3	32.2	31.1
2	2	4	23.1	-22.8
2	-2	4	19.7	-19.8
-2	2	4	31.6	31.8
2	2	5	13.4	12.8
2	2	-5	21.0	-26.7
2	-2	5	5.2	-4.4
-2	2	5	8.1	6.2
2	3	0	21.6	19.7
2	-3	0	8.9	7.2
2	3	1	40.2	-37.3
2	3	-1	31.1	28.9
2	-3	1	52.4	50.4
-2	3	1	40.4	38.9
2	3	2	56.7	52.9
2	3	-2	107.3	-122.8
2	-3	2	42.7	43.9
-2	3	2	22.3	-20.6
2	3	3	17.3	15.9
2	3	-3	8.6	-6.5
2	-3	3	44.3	44.1
-2	3	3	5.5	3.7
2	3	4	5.9	7.0
2	3	-4	22.4	-23.8
2	-3	4	4.5	5.8
-2	3	4	33.8	32.1
2	3	5	12.4	12.9
2	3	-5	33.4	-35.3
2	-3	5*	2.5	-.9
-2	3	5	12.4	-11.0
2	4	0	14.4	-13.6
2	-4	0	58.1	58.8
2	4	1	14.5	-15.6
2	4	-1	8.9	7.0
2	-4	1	12.2	10.3
-2	4	1	67.6	70.6
2	4	2	6.3	4.2
2	4	-2	24.3	-22.9
2	-4	2	38.3	37.5
-2	4	2	38.5	-33.7
2	4	3	29.7	31.4
2	4	-3	23.0	18.5
2	-4	3	30.5	28.5
-2	4	3	27.2	23.7
2	4	4	14.8	15.2
2	4	-4	12.3	-13.5
2	-4	4	6.6	-5.5
-2	4	4	20.9	-20.9
2	4	5	8.9	8.0
2	4	-5	29.3	-29.8
2	-4	5	13.9	13.2
-2	4	5	27.8	-25.5
2	5	0	57.8	59.1
2	-5	0	57.5	62.1
2	5	1	21.2	20.6
2	5	-1	9.9	8.2
2	-5	1	21.8	-21.7
-2	5	1	35.1	34.9
2	5	2	5.5	4.1
2	5	-2	17.7	-18.4
2	-5	2	11.2	9.9
-2	5	2	33.8	-30.9
2	5	3	30.4	32.3
2	5	-3	31.6	28.0
2	-5	3	33.9	31.6
-2	5	3	24.8	24.0
2	5	4*	3.0	-1.5
2	5	-4	23.5	-26.3
2	-5	4	7.7	7.0
-2	5	4	16.0	-15.0
2	5	5	8.9	8.2
2	5	-5	23.8	-22.5
2	-5	5	17.3	16.6
-2	5	5	24.4	-21.9
2	6	0	35.5	33.9
2	-6	0	39.2	-39.7
2	6	1	34.6	32.3
2	6	-1	29.5	29.6
2	-6	1	28.9	-26.7
-2	6	1	20.5	-18.4
2	6	2	27.0	26.6
2	6	-2	7.6	-7.0
2	-6	2	52.9	50.4
-2	6	2	69.4	-69.5
2	6	3	18.7	18.1
2	6	-3	16.7	15.7
2	-6	3	8.5	9.1
-2	6	3	20.0	-17.5
2	6	4*	3.0	-.3
2	6	-4	15.3	15.7
2	-6	4	8.5	8.8
-2	6	4	6.1	-6.0
2	6	5*	2.5	.3
2	6	-5	6.6	-4.6
2	-6	5	13.5	14.3
-2	6	5	21.1	-21.1
2	7	0	15.8	14.4
2	-7	0	20.0	-16.4
2	7	1	21.2	19.3
2	7	-1	34.3	33.6
2	-7	1	61.3	-67.8
-2	7	1*	2.8	-2.6
2	7	2*	2.9	-5.0
2	7	-2	47.5	46.1
2	-7	2	31.8	30.6
-2	7	2	68.1	-71.3
2	7	3	5.7	5.4
2	7	-3	20.4	19.9
2	-7	3	13.6	-12.7
-2	7	3	24.7	-24.3
2	7	4	4.8	-2.9
2	7	-4	33.7	35.6
2	-7	4	11.1	-9.6
-2	7	4	17.6	-19.1
2	7	5	10.8	-10.5
2	7	-5*	2.4	.6
2	-7	5	17.8	17.1
-2	7	5	16.8	-16.1
2	8	0	16.7	15.9
2	-8	0*	4.0	2.4
2	8	1	10.1	-10.1
2	8	-1*	3.3	.5
2	-8	1	59.5	-64.4
-2	8	1	11.6	-10.4
2	8	2	19.3	-18.7
2	8	-2	36.3	35.6
2	-8	2	20.9	-19.9
-2	8	2	7.9	-6.1
2	8	3	8.1	-8.5
2	8	-3	13.0	10.5
2	-8	3	14.2	-14.6
-2	8	3	7.6	7.1
2	8	4	18.7	-20.7
2	8	-4*	2.8	1.7
2	-8	4	19.8	-20.4
-2	8	4	7.6	7.3
2	8	5	5.1	-6.4
2	8	-5	10.0	9.9
2	-8	5	8.9	7.1
-2	8	5	6.1	6.4
2	9	0*	4.7	-6.1
2	-9	0	35.9	-35.6
2	9	1	29.4	-31.9
2	9	-1	19.0	-19.3
2	-9	1	14.6	-13.2
-2	9	1	16.7	-15.8
2	9	2*	3.0	-4.7
2	9	-2	22.3	-22.3
2	-9	2	14.2	-14.5
-2	9	2	15.4	15.0
2	9	3	14.1	-15.2
2	9	-3	15.3	14.0
2	-9	3	26.8	-26.1
-2	9	3*	2.8	1.7
2	9	4	11.8	-13.8
2	9	-4	17.9	19.3
2	-9	4	18.5	-18.4
-2	9	4	25.2	26.3
2	9	-5	14.8	14.3
2	-9	5	8.1	-8.2
-2	9	5	11.2	11.4
2	10	0	18.5	-18.8
2	-10	0	8.7	9.7
2	10	1	20.9	-21.6
2	10	-1	7.8	-6.4
2	-10	1*	3.6	1.3
-2	10	1	23.1	23.8
2	10	2*	2.9	-5.4
2	10	-2	16.5	-15.2
2	-10	2	6.3	5.8
-2	10	2*	3.0	.7
2	10	3	7.1	-7.8
2	10	-3*	2.8	-1.2
2	-10	3	13.6	-12.7
-2	10	3*	2.9	.0
2	10	4*	2.3	1.2
2	10	-4	12.5	11.0
2	-10	4	19.8	-19.5
-2	10	4	11.3	11.1
2	10	-5*	2.7	-2.1
2	-10	5*	2.8	-5.5
-2	10	5*	2.2	.5
2	11	0*	4.9	-2.0
2	-11	0	19.4	19.2
2	11	1	10.2	-10.0
2	11	-1	13.5	-12.0
2	-11	1*	3.8	3.4
-2	11	1	15.9	15.2
2	11	2	5.9	-6.4
2	11	-2	9.9	-9.3
2	-11	2*	3.0	-3.7
-2	11	2	21.3	21.3
2	11	3*	2.4	.7
2	11	-3	15.0	-15.3
2	-11	3	8.2	7.4
-2	11	3	16.3	18.2
2	11	-4	23.8	-26.7
2	-11	4	8.4	-8.3
-2	11	4	5.7	5.0
2	11	-5	7.7	-8.0
2	-11	5*	2.7	.7
-2	11	5	5.8	6.5
2	12	0*	4.7	.7
2	-12	0*	4.9	2.2
2	12	1	9.3	-8.4
2	12	-1	11.1	-11.6
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2	12	2	5.3	5.9
2	12	-2	27.6	-30.2
2	-12	2*	3.0	3.3
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2	12	3*	1.9	2.5
2	12	-3*	2.8	-.3
2	-12	3	13.0	13.7
-2	12	3	6.2	6.2
2	12	-4	10.6	-10.4
2	-12	4	8.1	7.5
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2	12	-5	6.8	-5.8
2	-12	5	6.1	-4.4
2	13	0	8.1	-8.8
2	-13	0	13.4	14.4
2	13	1*	3.2	2.9
2	13	-1	6.0	5.3
2	-13	1	18.8	18.3
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2	13	2	5.3	6.1
2	13	-2	7.4	-6.1
2	-13	2	17.8	19.5
-2	13	2*	2.8	-5.0
2	13	-3*	2.6	-.0
2	-13	3*	2.8	3.9
-2	13	3*	2.5	.0
2	13	-4*	3.0	2.3
2	-13	4*	2.9	2.9
-2	13	4*	1.7	-1.3
2	13	-5	9.2	-9.7
2	-13	5*	2.0	2.1
2	14	0	8.3	9.2
2	-14	0	7.2	6.4
2	14	1	10.9	13.9
2	14	-1	7.5	7.9
2	-14	1	4.7	-4.2
-2	14	1*	3.1	1.5
2	14	-2	7.0	8.7
2	-14	2	6.9	6.8
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2	14	-3	4.8	-5.4
2	-14	3	7.9	8.1
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2	14	-4	6.8	-7.9
2	-14	4	7.2	8.2
2	14	-5*	1.7	-8.1
2	-15	0	7.0	-7.1
2	15	-1	5.2	5.2
2	-15	1*	3.1	-2.5
-2	15	1	11.6	-14.3
2	-15	2	4.6	4.5
-2	15	2	8.2	-10.9
2	15	-3*	2.0	3.0
2	-16	0*	2.4	-7.1
2	-16	1	4.7	-3.7
3	0	0	15.6	18.7
3	0	1	31.7	32.2
3	0	-1*	1.5	-1.9
3	0	2	11.8	-10.2
3	0	-2	6.0	-5.7
3	0	3	14.3	13.2
3	0	4	17.1	16.6
3	0	5	7.6	6.0
3	1	0*	2.5	-2.2
3	-1	0	16.2	-18.9
3	1	1	11.3	-12.0
3	1	-1	36.0	-35.0
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-3	1	1	43.0	47.2
3	1	2*	2.2	2.6
3	1	-2	27.3	-26.0
3	-1	2	13.2	11.2
-3	1	2	27.6	28.3
3	1	3	25.6	26.4
3	1	-3	2.7	2.2
3	-1	3	5.3	-4.8
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3	1	4	8.4	-6.1
3	-1	4	8.9	7.2
-3	1	4	10.6	12.2
3	1	5*	2.8	2.9
3	-1	5	12.5	13.4
-3	1	5	5.9	-6.6
3	2	0	9.6	7.4
3	-2	0*	2.4	-2.3
3	2	1	27.4	-27.2
3	2	-1	27.5	23.9
3	-2	1	17.9	-21.5
-3	2	1	49.9	-52.1
3	2	2	12.4	10.9
3	2	-2	7.6	-7.6
3	-2	2	6.3	-5.3
-3	2	2	4.3	-3.1
3	2	3	5.6	4.5
3	2	-3	43.0	46.3
3	-2	3*	2.2	2.0
-3	2	3	6.9	3.5
3	2	4	7.0	-7.3
3	-2	4	12.3	-9.6
-3	2	4	4.2	-3.1
3	2	5	5.9	4.8
3	-2	5*	2.6	-2.4
-3	2	5	20.4	21.5
3	3	0	19.5	20.6
3	-3	0*	2.5	2.9
3	3	1	19.6	18.7
3	3	-1*	2.0	-2.8
3	-3	1	9.3	12.4
-3	3	1	20.7	18.5
3	3	2	6.7	-3.9
3	3	-2	22.3	-18.2
3	-3	2	18.7	-19.8
-3	3	2	21.3	20.1
3	3	3*	2.6	-2.3
3	3	-3	18.9	-19.8
3	-3	3	17.1	-17.6
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3	3	4*	3.0	1.5
3	3	-4	19.3	-23.1
3	-3	4*	2.7	-.7
-3	3	4	6.2	6.7
3	3	5*	2.7	-4.4
3	3	-5	28.3	-35.7
3	-3	5	13.3	-12.8
-3	3	5	3.2	3.2
3	4	0	23.1	23.5
3	-4	0	35.7	-36.9
3	4	1	6.5	-5.3
3	4	-1	38.5	-36.6
3	-4	1	4.5	-5.7
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3	4	2	11.9	-12.8
3	4	-2	16.9	-16.6
3	-4	2	9.6	8.4
-3	4	2	4.3	2.1
3	4	3	16.7	17.9
3	4	-3	17.8	-16.1
3	-4	3	28.7	-28.8
-3	4	3*	1.9	-3.5
3	4	4	6.3	-5.4
3	4	-4	12.6	-12.0
3	-4	4	9.0	6.4
-3	4	4	21.8	19.6
3	4	5	7.9	-8.0
3	4	-5	9.9	9.6
3	-4	5*	2.7	-1.7
-3	4	5	20.7	-20.9
3	5	0	11.9	10.5
3	-5	0	5.8	-4.7
3	5	1	24.5	-25.9
3	5	-1	18.8	-18.0
3	-5	1	4.0	2.9
-3	5	1	22.6	-20.6
3	5	2	6.4	-7.1
3	5	-2	9.7	8.9
3	-5	2	15.6	15.8
-3	5	2	4.7	-1.6
3	5	3*	2.8	2.7
3	5	-3	41.4	39.1
3	-5	3	3.7	-3.0
-3	5	3	4.5	4.1
3	5	4	7.0	-7.2
3	5	-4	9.6	-9.5
3	-5	4	8.5	-7.7
-3	5	4	10.5	-9.1
3	5	5	4.8	-5.4
3	5	-5	8.9	-8.3
3	-5	5	6.2	-6.6
-3	5	5*	2.4	-3.5
3	6	0	8.8	8.9
3	-6	0*	3.4	-2.6
3	6	1	16.2	15.5
3	6	-1	10.5	8.5
3	-6	1	22.8	23.3
-3	6	1	24.8	23.6
3	6	2	9.0	-8.4
3	6	-2	15.0	12.7
3	-6	2	14.7	-14.4
-3	6	2	30.8	29.6
3	6	3	9.6	-11.0
3	6	-3	8.8	-8.4
3	-6	3	15.0	-13.9
-3	6	3	37.9	-38.0
3	6	4*	3.0	-.7
3	6	-4	13.1	-12.6
3	-6	4	9.6	-9.1
-3	6	4	12.4	-12.0
3	5	5	8.5	-8.6
3	6	-5	17.0	-16.2

TABLE I (*continued*).

h	*k*	*l*	F_O	F_C
3	-6	5	10.6	-11.8
-3	6	5	9.2	9.7
3	7	0	15.8	16.3
3	-7	0	20.6	-21.4
3	7	1	17.8	18.7
3	7	-1	26.0	-25.3
3	-7	1	15.1	14.4
-3	7	1•	2.8	1.7
3	7	2	13.6	-14.1
3	7	-2	9.1	8.2
3	-7	2	5.2	-5.0
-3	7	2	5.0	-4.1
3	7	3	9.2	9.7
3	7	-3	7.6	-6.2
3	-7	3	5.3	-5.3
-3	7	3	6.6	-6.5
3	7	4•	2.9	3.4
3	7	-4	9.6	-8.1
3	-7	4	16.2	16.0
-3	7	4	12.8	11.7
3	7	5	4.6	-4.2
3	7	-5	14.8	14.3
3	-7	5•	2.8	4.3
-3	7	5	5.8	-3.8
3	8	0•	4.6	3.7
3	-8	0	5.0	5.4
3	8	1	15.5	-16.6
3	8	-1	8.8	-8.8
3	-8	1	20.7	21.2
-3	8	1•	3.2	-12.8
3	8	2•	3.0	-5.9
3	8	-2	10.8	10.7
3	-8	2	29.8	30.5
-3	8	2	5.3	-3.1
3	8	3	8.0	8.4
3	8	-3	37.5	34.7
3	-8	3	25.0	25.5
-3	8	3	11.6	12.6
3	8	4•	2.7	.5
3	8	-4	6.2	5.2
3	-8	4	12.0	11.8
-3	8	4	6.6	-6.1
3	8	-5	14.8	14.8
3	-8	5	10.1	9.9
-3	8	5	8.4	8.6
3	9	0•	4.8	-.6
3	-9	0	6.3	5.2
3	9	1•	3.8	1.5
3	9	-1	18.7	16.7
3	-9	1	18.3	17.3
-3	9	1•	3.4	-.6
3	9	2•	3.0	.2
3	9	-2	9.9	9.6
3	-9	2	7.0	-6.7
-3	9	2	21.6	21.3
3	9	3•	2.7	-3.4
3	9	-3	11.0	10.7
3	-9	3•	2.8	1.7
-3	9	3	10.4	-11.1
3	9	4•	2.1	1.3
3	9	-4	6.4	6.7
3	-9	4•	3.0	4.1
-3	9	4	10.0	-9.6
3	9	-5•	2.6	3.8
3	-9	5	6.3	5.1
-3	9	5	14.2	14.4
3	10	0•	4.9	5.0
3	-10	0	21.0	-21.4
3	10	1	11.1	11.6
3	10	-1	19.4	-18.7
3	-10	1	10.9	-9.7
-3	10	1•	3.6	3.3
3	10	2•	2.9	-4.2
3	10	-2	7.7	-7.7
3	-10	2	14.2	-14.0
-3	10	2•	3.0	3.7
3	10	3	5.7	7.0
3	10	-3	5.0	-3.2
3	-10	3	7.2	-7.4
-3	10	3•	2.9	-5.9
3	10	4•	1.2	1.4
3	10	-4	5.4	-3.7
3	-10	4	15.7	15.7
-3	10	4	10.3	10.5
3	10	-5	8.4	9.9
3	-10	5	6.7	7.8
-3	10	5•	2.3	-.9
3	11	0•	4.8	5.1
3	-11	0	11.5	-10.8
3	11	1	12.4	-12.8
3	11	-1	13.8	-14.0
3	-11	1•	3.8	-1.5
-3	11	1•	3.8	-4.8
3	11	2•	2.8	-3.3
3	11	-2	9.6	-10.0
3	12	0•	4.6	3.6
3	-12	0•	4.9	1.7
3	12	1•	3.1	-4.3
3	12	-1	6.9	5.7
3	-12	1	9.3	8.4
-3	12	1•	3.8	-4.8
3	12	2•	2.3	.1
3	12	-2•	2.9	-2.0
3	-12	2	6.0	-6.2
-3	12	2	8.3	8.0
3	12	-3•	2.9	2.9
3	-12	3	12.9	-12.4
-3	12	3	5.8	-6.8
3	12	-4	9.9	-11.3
3	-12	4	5.9	-6.2
-3	12	4	4.6	-4.4
3	12	-5	11.6	-12.9
3	-12	5	6.7	-7.6
-3	12	5•	1.2	4.1
3	13	0•	4.1	.8
3	-13	0	17.2	-18.1
3	13	1	6.0	7.6
3	13	-1	11.4	-11.3
3	-13	1	5.1	-3.4
-3	13	1	8.8	8.8
3	13	-2•	2.7	-2.4
3	-13	2	12.0	-12.7
-3	13	2	13.4	15.0
3	13	-3	7.2	-7.3
3	-13	3	12.9	-15.1
-3	13	3	6.4	-7.1
3	13	-4	5.8	-6.7
3	-13	4•	2.8	1.8
-3	13	4	5.0	5.8
3	13	-5•	2.3	-.1
3	-13	5•	1.6	-5.1
3	14	0•	3.3	4.1
3	-14	0	8.5	-9.5
3	14	-1	9.8	-10.8
3	-14	1•	3.6	.6
-3	14	1•	3.1	-.8
3	14	-2•	2.3	.7
3	-14	2•	2.8	.2
-3	14	2•	2.6	-4.0
3	14	-3•	2.3	2.4
3	-14	3	8.3	-9.5
-3	14	3•	1.9	-.6
3	14	-4	5.2	-6.1
3	-14	4•	2.2	-.2
3	14	-5•	1.4	.3
3	-15	0	9.9	10.9
3	15	-1•	1.5	5.3
3	-15	1	13.0	13.9
-3	15	1•	2.5	-2.9
3	15	-2•	1.6	2.7
3	-15	2•	2.3	1.5
-3	15	2•	2.1	2.9
3	15	-3•	1.6	.8
3	-15	3•	2.0	.6
3	-16	0•	2.9	.1
3	-16	1	8.2	9.3
4	0	0	19.5	-20.1
4	0	1	27.3	-26.8
4	0	-1	95.8	-94.5
4	0	2	4.8	5.6
4	0	-2	23.2	-22.3
4	0	3	24.5	24.5
4	0	-3	40.6	-44.9
4	0	4	8.5	6.9
4	0	5	22.0	21.1
4	1	0	57.7	61.2
4	-1	0	62.3	-64.2
4	1	1•	2.5	-2.8
4	1	-1•	2.0	.6
4	-1	1	39.2	-44.3
-4	1	1	14.8	-10.9
4	1	2	35.5	35.5
4	1	-2	10.7	-9.8
4	-1	2	11.1	11.0
-4	1	2	59.8	-61.6
4	1	3	12.9	10.8
4	1	-3	15.9	-18.8
4	-1	3•	2.5	3.0
-4	1	3	63.4	-63.3
4	1	4•	3.0	3.0
4	-1	4	8.4	-5.4
-4	1	4	20.2	26.1
4	1	5	18.9	18.9
4	-1	5	12.1	11.7
-4	1	5	10.1	-18.4
4	2	0	34.5	32.3
4	-2	0	19.3	-17.0
4	2	1	30.9	30.1
4	2	-1	64.3	66.9
4	-2	1	52.4	-55.0
-4	2	1	46.5	50.8
4	2	2	55.8	56.1
4	2	-2	4.7	-5.7
4	-2	2	18.0	-16.0
-4	2	2	60.0	-57.5
4	2	3	4.8	4.2
4	2	-3	23.9	-19.8
4	-2	3	29.5	-29.7
-4	2	3	6.6	-5.3
4	2	4	11.6	12.7
4	2	-4	16.9	19.9
4	-2	4	27.5	-28.1
-4	2	4	21.1	19.9
4	2	5	6.3	6.2
4	-2	5	7.7	6.9
-4	2	5	22.2	-24.3
4	3	0	9.6	-6.9
4	-3	0	60.5	-61.5
4	3	1	14.6	13.9
4	3	-1	44.6	42.7
4	-3	1	36.6	-37.0
-4	3	1	39.3	39.2
4	3	2	26.4	25.2
4	3	-2	51.4	49.6
4	-3	2	12.5	-12.9
-4	3	2	25.9	-24.0
4	3	3•	2.8	-.5
4	3	-3	20.5	20.0
4	-3	3	24.8	-25.8
-4	3	3	13.2	12.1
4	3	4	7.9	7.7
4	3	-4	18.4	17.3
4	-3	4	23.0	-23.8
-4	3	4	42.0	43.7
4	3	5•	2.7	.6
4	3	-5	7.0	7.5
4	-3	5•	2.6	-.8
-4	3	5	5.5	3.6
4	4	0	10.0	8.2
4	-4	0	82.1	-84.9
4	4	1	12.1	-10.1
4	4	-1	58.3	56.9
4	-4	1	6.7	5.2
-4	4	1	55.8	55.5
4	4	2	20.0	19.8
4	4	-2	8.9	-9.3
4	-4	2	29.4	27.2
-4	4	2	15.9	-14.9
4	4	3	13.0	-13.0
4	4	-3	41.5	37.7
4	-4	3	31.0	-29.4
-4	4	3	13.8	-10.9
4	4	4	10.1	-10.8
4	4	-4	24.0	21.5
4	-4	4	8.7	-6.4
-4	4	4	52.1	54.6
4	4	5•	2.5	-.6
4	4	-5•	1.7	1.5
4	-4	5	7.6	-7.6
-4	4	5	13.3	11.6
4	5	0	15.4	-12.2
4	-5	0	9.3	7.7
4	5	1•	3.3	-3.0
4	5	-1	56.5	56.9
4	-5	1	4.8	4.9
-4	5	1	93.1	99.5
4	5	2	14.6	14.1
4	5	-2	39.5	-37.6
4	-5	2	37.1	36.9
-4	5	2•	2.1	3.0
4	5	3	18.8	-20.1
4	5	-3	8.1	10.5
4	-5	3	33.6	-33.5
-4	5	3	12.7	11.2
4	5	4	9.9	-10.5
4	5	-4	47.0	49.8
4	-5	4	4.9	-4.6
-4	5	4	27.4	27.3
4	5	5	7.1	-6.6
4	5	-5	3.7	3.7
4	-5	5•	3.4	-2.7
-4	5	5•	2.3	2.8
4	6	0	30.6	-29.4
4	-6	0	32.5	32.4
4	6	1	19.0	-18.4
4	6	-1	24.2	24.1
4	-6	1	11.9	8.3
-4	6	1	50.9	50.6
4	6	2	16.0	-17.0
4	6	-2	8.1	8.6
4	-6	2	29.1	27.8
-4	6	2	50.6	49.8
4	6	3	12.0	-11.8
4	6	-3	4.1	4.8
4	-6	3	11.3	-11.1
-4	6	3	35.3	35.3
4	6	4	12.5	-11.9
4	6	-4	34.5	37.3
4	-6	4•	3.0	2.5
-4	6	4	18.0	18.3
4	6	5	6.3	-7.2
4	6	-5•	2.2	1.4
4	-6	5	5.5	3.9
-4	6	5	12.2	11.4
4	7	0	13.6	-13.5
4	-7	0•	3.9	2.6
4	7	1	31.6	-30.1
4	7	-1	15.7	-14.1
4	-7	1	36.9	37.9
-4	7	1	10.1	-9.6
4	7	2	17.4	-18.4
4	7	-2	19.4	-19.8
4	-7	2	37.1	37.4
-4	7	2	19.2	17.1
4	7	3	5.5	-5.0
4	7	-3	5.6	-5.2
4	-7	3	7.9	8.6
-4	7	3	21.0	-19.8
4	7	4	13.0	-13.8
4	7	-4•	2.7	-4.2
4	-7	4	17.8	20.3
-4	7	4•	2.8	-2.3
4	7	-5	13.2	-13.6
4	-7	5	9.0	8.2
-4	7	5•	2.6	-1.8
4	8	0	19.8	-18.6
4	-8	0	16.5	17.5
4	8	1	18.0	-18.5
4	8	-1	27.1	-26.1
4	-8	1	13.7	13.6
-4	8	1	14.6	12.8
4	8	2•	3.0	-.4
4	8	-2	40.1	-43.2
4	-8	2	37.9	40.9
-4	8	2	21.5	-21.2
4	8	3•	2.7	-1.5
4	8	-3	22.3	-21.6
4	-8	3	13.8	14.1
-4	8	3	38.1	-38.9
4	8	4•	2.3	-.2
4	8	-4•	2.9	1.2
4	-8	4	13.0	12.9
-4	8	4	20.7	-20.6
4	8	-5	11.0	-10.4
4	-8	5	16.3	15.9
-4	8	5	21.2	-21.6
4	9	0•	4.9	-6.9
4	-9	0•	4.5	-3.6
4	9	1•	3.7	.5
4	9	-1	12.3	-10.9
4	-9	1	21.0	-22.0
-4	9	1	19.8	-18.2
4	9	2•	2.9	2.9
4	9	-2	5.5	-4.6
4	-9	2	6.9	-6.2
-4	9	2	6.1	-5.6
4	9	3	8.8	8.6
4	9	-3	19.4	-19.7
4	-9	3	10.5	8.8
-4	9	3•	2.8	-3.7
4	9	-4•	3.0	.6
4	-9	4•	3.1	2.0
-4	9	4	11.8	-10.9
4	9	-5	11.8	-11.0
4	-9	5	14.4	15.6
-4	9	5	7.9	-8.3
4	10	0	17.8	16.8
4	-10	0	30.3	-32.4
4	10	1	6.4	7.2
4	10	-1•	3.8	-.8
4	-10	1	9.9	-11.3
-4	10	1	30.6	-31.6
4	10	2	8.3	8.8
4	10	-2	7.0	7.0
4	-10	2	17.4	-16.7
-4	10	2	16.3	-16.1
4	10	3	7.8	9.9
4	10	-3	10.5	-10.2
4	-10	3•	2.9	.3
-4	10	3	19.6	-21.5
4	10	-4	25.3	-27.7
4	-10	4•	3.1	-1.6
-4	10	4•	3.2	3.7
4	10	-5	12.8	-13.0
4	-10	5	3.9	4.2
-4	10	5•	2.5	-.5
4	11	0	10.1	10.5
4	-11	0	23.2	-22.8
4	11	1•	3.4	3.9
4	11	-1	6.9	6.7
4	-11	1	8.7	-6.9
-4	11	1	9.3	9.9
4	11	2	11.1	13.9
4	11	-2	6.7	-7.1
4	-11	2•	3.0	.0
-4	11	2	19.7	-19.8
4	11	-3	5.1	4.4
4	-11	3	16.1	-15.5
-4	11	3	17.6	-18.2
4	11	-4•	3.1	-3.0
4	-11	4	10.2	-10.2
-4	11	4•	2.8	2.7
4	11	-5•	2.7	-.9
4	-11	5•	2.3	.5
-4	11	5	9.0	-9.1
4	12	0•	4.3	.0
4	-12	0	13.1	-12.2
4	12	1	6.1	7.0
4	12	-1	15.3	14.0
4	-12	1	21.8	-21.7
-4	12	1•	3.8	4.8
4	12	-2	8.5	9.0
4	-12	2	13.6	-14.4
-4	12	2•	3.0	-3.3
4	12	-3	9.5	10.5
4	-12	3	13.2	-13.1
-4	12	3	10.1	11.5
4	12	-4	14.3	16.6
4	-12	4	7.7	-8.7
-4	12	4	4.6	4.1
4	12	-5•	2.5	3.3
4	-12	5•	1.8	-2.8
-4	12	5	4.0	4.9
4	13	0	7.4	8.9
4	-13	0	9.7	-9.0
4	13	1	4.7	6.4
4	13	-1	10.5	10.9
4	-13	1•	3.6	-.3
-4	13	1•	3.6	1.0
4	13	-2	11.2	13.1
4	-13	2•	2.9	-3.0
-4	13	2	6.8	6.9
4	13	-3	4.8	6.2
4	-13	3	7.6	-7.4
-4	13	3	6.4	7.3
4	13	-4•	2.4	-1.4
4	-13	4	4.7	-5.6
-4	13	4	14.8	15.8
4	14	0•	2.2	2.4
4	-14	0•	4.5	5.8
4	-14	1	11.7	10.8
-4	14	1	18.6	20.2
4	14	-2•	2.0	-2.6
4	-14	2	6.6	5.8
-4	14	2	9.8	10.9
4	14	-3•	2.1	6.3
4	-14	3	12.6	-12.4
4	14	-4	4.3	5.4
4	-14	4•	1.8	-2.8
4	-15	0	12.8	13.8
4	-15	1•	2.8	1.6
-4	15	1	12.4	14.2
4	-15	2	8.9	8.7
-4	15	2	7.6	8.5
4	-15	3•	1.9	3.1
4	-16	1•	2.3	11.2
5	0	0	9.4	11.2
5	0	1	13.8	-14.9
5	0	-1	27.6	-27.2
5	0	2•	2.6	2.7
5	0	-2	34.3	-33.5
5	0	3	10.3	11.2
5	0	-3	3.5	-1.8
5	0	4	11.1	-9.7
5	0	-4	19.8	-21.5
5	0	5	5.7	-5.0
5	1	0	12.2	-12.7
5	-1	0	24.7	22.7
5	1	1	12.3	-12.5
5	1	-1	12.2	8.9
5	-1	1	21.9	23.8
-5	1	1	5.3	5.0
5	1	2•	2.7	-1.1
5	1	-2•	2.6	-.3
5	-1	2•	2.5	-1.3
-5	1	2	7.8	7.0
5	1	3	10.3	-10.0
5	1	-3	24.1	22.7
5	-1	3	11.8	9.7
-5	1	3	27.2	-27.0
5	1	4	10.9	-11.2
5	1	-4	7.7	-8.1
5	-1	4	8.0	6.9
-5	1	4	7.5	-8.1
5	1	5•	2.5	-3.4
5	-1	5•	2.7	-2.9
-5	1	5•	2.7	2.8
5	2	0	17.4	16.8
5	-2	0	19.3	-16.8
5	2	1	9.5	10.1
5	2	-1	18.3	17.8
5	-2	1	9.2	6.8
-5	2	1	7.1	7.0
5	2	2	12.4	-10.3
5	2	-2	3.7	2.2
5	-2	2	12.2	13.2
-5	2	2	21.7	20.5
5	2	3•	2.8	-2.1
5	2	-3	11.9	-10.4
5	-2	3•	2.7	-.9
-5	2	3	19.3	17.5
5	2	4	6.2	-5.6
5	2	-4	14.5	-14.8
5	-2	4	14.4	13.3
-5	2	4	19.9	19.4
5	2	5	3.9	-3.6
5	2	-5	23.1	-28.7
-5	2	5	3.9	-10.8
5	3	0	7.9	7.6
5	-3	0	6.1	5.4
5	3	1	12.2	-10.0
5	3	-1	18.5	-17.2
5	-3	1	14.5	-13.3
-5	3	1	13.6	-13.0
5	3	2•	2.9	-.9
5	3	-2	19.1	-16.8
5	-3	2	10.8	9.8
-5	3	2	9.3	-7.3
5	3	3	6.9	7.4
5	3	-3	3.7	2.7
5	-3	3	7.4	8.9
-5	3	3•	1.8	1.4
5	3	4	8.0	-7.6
5	3	-4•	1.8	-2.0
5	-3	4•	3.1	4.5
-5	3	4•	1.9	-.5
5	3	5•	2.3	1.4
5	3	-5	10.6	11.4
5	-3	5	6.3	6.5
-5	3	5	14.9	15.2
5	4	0•	4.1	-6.3
5	-4	0	7.8	5.5
5	4	1	22.8	-25.1
5	4	-1	19.1	17.2
5	-4	1	14.2	14.3
-5	4	1	13.0	-11.1
5	4	2	7.9	7.7
5	4	-2	8.5	-9.0
5	-4	2	11.3	-11.2
-5	4	2	19.9	18.2
5	4	3•	2.8	-3.4
5	4	-3	29.8	27.8
5	-4	3•	2.7	.4
-5	4	3	29.9	-29.8
5	4	4	4.8	-4.9
5	4	-4	24.7	25.1
5	-4	4	5.9	5.5
-5	4	4	5.1	-5.7
5	4	-5	5.8	-6.7
5	-4	5•	2.7	3.5
-5	4	5	17.0	16.4
5	5	0•	4.3	5.0
5	-5	0	18.3	-16.0
5	5	1•	3.6	-.0
5	5	-1	20.7	21.1
5	-5	1•	3.0	-1.5
-5	5	1•	2.6	1.0
5	5	2•	3.0	2.3
5	5	-2•	2.4	1.9
5	-5	2	4.5	-2.6
-5	5	2•	2.2	2.3
5	5	3•	2.8	-3.8
5	5	-3•	2.2	3.8
5	-5	3•	2.7	-2.9
-5	5	3	13.0	11.9
5	5	4•	2.7	.6
5	5	-4	13.2	12.5
5	-5	4	9.9	9.0
-5	5	4	21.7	20.9
5	5	5•	1.2	1.4
5	5	-5	21.4	-20.5
5	-5	5	4.9	4.5
-5	5	5	10.0	-9.7
5	6	0	17.2	17.6
5	-6	0•	3.8	-.5
5	6	1•	3.7	-4.7
5	6	-1	10.5	-9.6
5	-6	1	8.5	-7.5
-5	6	1	7.2	-5.9
5	6	2•	3.2	2.9
5	6	-2	13.3	-13.9
5	-6	2•	2.7	-.1
-5	6	2•	2.3	-3.7
5	6	3	9.5	10.4
5	6	-3	4.3	3.3
5	-6	3•	2.8	-4.0
-5	6	3	22.9	22.3
5	6	4•	2.4	.4
5	6	-4	5.5	4.3
5	-6	4	9.5	-9.2
-5	6	4	9.2	-9.4
5	6	-5	10.2	8.8
5	-6	5•	2.6	.7
-5	6	5•	2.5	1.8
5	7	0	8.2	7.7
5	-7	0•	4.1	-1.8
5	7	1	18.3	-20.7
5	7	-1•	3.6	.7
5	-7	1•	3.3	-1.3
-5	7	1	9.5	-9.7
5	7	2•	3.1	5.5
5	7	-2	15.1	-16.1
5	-7	2	25.4	-26.8
-5	7	2	13.8	13.4
5	7	3	6.8	8.0
5	7	-3	28.8	28.1
5	-7	3	13.0	-12.6
-5	7	3	13.0	-12.8
5	7	4•	2.0	.0
5	7	-4	9.7	9.5
5	-7	4	14.0	-13.4
-5	7	4	22.0	-22.4
5	7	-5•	2.5	-.3
5	-7	5	7.2	-8.7
-5	7	5	9.0	9.3
5	8	0•	4.9	.1
5	-8	0	11.3	-9.8
5	8	1•	3.8	-2.4
5	8	-1•	3.7	2.3
5	-8	1	5.1	4.0
-5	8	1•	3.3	5.9
5	8	2•	2.8	-.7
5	8	-2•	3.0	-4.4
5	-8	2	11.7	-11.9
-5	8	2•	2.7	4.1
5	8	3•	2.4	1.0
5	8	-3•	2.8	3.6
5	-8	3	5.5	-6.6
-5	8	3	8.2	-7.6
5	8	-4•	3.0	-3.8
5	-8	4•	3.1	.3
-5	8	4	5.6	5.0
5	8	-5	8.9	-7.1
5	-8	5	9.7	-9.8
-5	8	5	6.3	-6.1
5	9	0	12.3	12.3
5	-9	0•	4.6	2.6
5	9	1•	3.6	4.3
5	9	-1	18.0	-17.7
5	-9	1	21.8	23.0
-5	9	1•	3.6	-5.3
5	9	2	5.5	-4.8
5	9	-2	10.7	-11.3
5	-9	2	12.1	11.9
-5	9	2•	2.9	3.1
5	9	3	5.8	6.4
5	9	-3	6.5	-6.5
5	-9	3•	2.9	-1.4
-5	9	3	8.3	7.4
5	9	-4	15.8	-17.0
5	-9	4•	3.1	1.4
-5	9	4•	3.0	-4.1
5	9	-5•	2.7	2.0
5	-9	5	7.6	-7.9
-5	9	5•	2.7	3.5
5	10	0	6.5	-7.4
5	-10	0	10.5	9.3
5	10	1	8.0	-8.7
5	10	-1	6.3	-5.6
5	-10	1	14.4	13.4
-5	10	1•	3.7	-8.2
5	10	2•	2.5	-.8
5	10	-2	10.5	-10.6
5	-10	2	6.0	-5.5
-5	10	2	22.8	17.0
5	10	-3	9.2	8.9
5	-10	3•	2.9	4.9
-5	10	3	7.3	-7.6
5	10	-4	12.0	-13.0
5	-10	4	5.2	5.0
-5	10	4	14.1	-14.3
5	10	-5	8.7	-9.2
5	-10	5	5.2	-5.6
-5	10	5	8.9	9.4
5	11	0•	4.5	-.7
5	-11	0•	4.9	-5.6
5	11	1•	3.1	-1.4
5	11	-1	8.1	7.9
5	-11	1	10.2	11.3
-5	11	1•	3.8	-2.2
5	11	2•	1.9	-.1
5	11	-2•	2.9	1.6
5	-11	2	6.2	-6.7
-5	11	2	15.7	17.8
5	11	-3•	2.8	1.4
5	-11	3	6.3	5.2
-5	11	3	9.5	-8.6
5	11	-4•	3.0	-4.2
5	-11	4	14.9	16.5
-5	11	4•	3.0	1.1
5	11	-5	11.7	-12.5
5	-11	5•	1.8	2.1
-5	11	5•	2.4	2.6
5	12	0•	4.0	3.6
5	-12	0•	4.9	.5
5	12	1•	2.4	3.6
5	12	-1•	3.1	-2.8
5	-12	1	12.8	11.9
-5	12	1	12.1	-12.9
5	12	-2•	2.9	.8
5	-12	2	5.3	5.6
-5	12	2	6.2	-5.7
5	12	-3•	2.6	-.4
5	-12	3	5.6	7.1
-5	12	3•	2.8	2.0
5	12	-4•	2.7	1.6
5	-12	4	10.2	11.7
-5	12	4•	3.2	1.6
5	12	-5•	2.3	1.8
-5	12	5•	2.7	2.5
5	13	0•	2.9	4.5
5	-13	0	9.9	11.3
5	-13	1•	3.7	3.7
-5	13	1	8.4	-9.0
5	13	-2•	2.3	-2.4
5	-13	2•	2.8	-1.8
-5	13	2•	2.9	2.7
5	13	-3	7.0	9.1
5	-13	3	6.8	7.7
-5	13	3•	2.4	2.0
5	13	-4•	2.4	2.8
5	-13	4•	2.8	1.5
-5	13	4	9.3	-10.2
5	-14	0	7.0	-6.8
5	-14	1•	3.4	-3.9
-5	14	1•	3.4	-5.6
5	14	-2•	1.5	-.0
5	-14	2	12.2	-14.0
-5	14	2	9.1	11.7
5	14	-3•	3.0	4.3
5	-14	3•	2.1	-1.8
-5	14	3•	2.2	1.3
5	14	-4•	1.4	2.7
5	-15	0	6.9	-9.0
5	-15	1	8.5	-9.0
-5	15	1•	2.8	-6.4
5	-15	2	5.4	-5.5
5	-16	0•	2.7	8.0
6	0	0	23.1	22.4
6	0	1	29.7	29.2
6	0	-1	55.9	61.3
6	0	2	24.7	24.8
6	0	-2	28.8	27.5
6	0	3	6.0	-6.5
6	0	-3	14.4	-12.9
6	0	4•	3.2	-.5
6	0	-4	32.2	33.8
6	0	5	5.0	4.5
6	0	-5	12.5	-14.8
6	1	0•	3.9	.8
6	-1	0	28.2	-27.8
6	1	1	10.3	9.7
6	1	-1	56.2	63.5
6	-1	1	45.7	49.0
-6	1	1	16.9	15.6
6	1	2	17.5	16.6
6	1	-2	49.2	50.8
6	-1	2	26.1	25.5
-6	1	2	47.5	45.3
6	1	3	16.2	-16.7
6	1	-3	15.7	-12.3
6	-1	3	12.4	13.8
-6	1	3	53.9	-41.7
6	1	4	8.8	-6.6
6	1	-4	73.4	63.1
6	-1	4	15.5	13.7
-6	1	4	14.5	10.5
6	1	5	5.3	-4.3
6	1	-5	31.0	21.4
6	-1	5	12.2	9.8
-6	1	5	6.0	-4.2
6	2	0	10.5	-10.6
6	-2	0	51.4	-47.9
6	2	1	21.6	-21.0
6	2	-1•	2.8	-1.3
6	-2	1	46.2	53.5
-6	2	1	19.9	16.9
6	2	2•	3.0	-2.0
6	2	-2	34.9	33.0
6	-2	2	16.3	15.3
-6	2	2	15.1	14.9
6	2	3	14.0	-14.4
6	2	-3	20.7	18.0
6	-2	3	6.3	6.4
-6	2	3	71.8	-72.9
6	2	4	10.8	-10.2
6	2	-4	28.3	28.3
6	-2	4	22.2	23.6
-6	2	4	0.6	8.2
6	2	5•	2.0	-3.9
6	2	-5	26.7	27.6
6	-2	5	7.4	7.1
-6	2	5•	3.2	-4.2
6	3	0	11.7	-10.2
6	-3	0	37.5	-36.1
6	3	1	31.7	-32.7
6	3	-1	11.5	-9.9
6	-3	1	22.7	23.0
-6	3	1	18.2	17.4
6	3	2•	3.0	-3.1
6	3	-2	24.9	-22.5
6	-3	2•	2.8	.5
-6	3	2	18.5	-18.6
6	3	3	18.5	-20.7
6	3	-3	14.1	11.6
6	-3	3	11.9	-11.8
-6	3	3	39.6	-40.2
6	3	4	8.4	-8.7
6	3	-4	4.3	-3.4
6	-3	4	17.2	16.4
-6	3	4	17.6	-18.3
6	3	5•	1.3	-1.0
6	3	-5	9.8	8.7
6	-3	5	6.8	6.9
-6	3	5	17.2	-16.3
6	4	0	32.1	-30.3
6	-4	0	44.0	-44.1
6	4	1	8.5	-12.1
6	4	-1•	3.2	-.5
6	-4	1	11.7	-7.8
-6	4	1	30.2	-30.1
6	4	2•	3.0	-3.0
6	4	-2	32.1	-30.8
6	-4	2	11.1	-10.9
-6	4	2	11.3	-10.6
6	4	3	16.6	-17.8
6	4	-3	22.2	-22.1
6	-4	3	13.0	-12.6
-6	4	3	12.7	-11.5
6	4	4•	2.6	-.3
6	4	-4	9.6	7.7
6	-4	4	10.3	9.7
-6	4	4	27.5	-27.7
6	4	-5	10.9	11.5
6	-4	5	4.6	3.0
-6	4	5	8.0	6.5
6	5	0	30.1	-29.1
6	-5	0	42.1	-42.2
6	5	1•	3.8	-2.5
6	5	-1	14.8	-12.0
6	-5	1	10.2	-8.1
-6	5	1	41.6	-45.1
6	5	2	9.5	-10.1
6	5	-2	5.3	-4.7
6	-5	2	8.8	-8.6
-6	5	2	29.5	-29.1
6	5	3	4.4	-4.4
6	5	-3	21.3	-17.2
6	-5	3	18.7	-17.6
-6	5	3	29.3	-30.4
6	5	4•	2.4	4.3
6	5	-4	12.2	-11.3
6	-5	4	5.9	5.9
-6	5	4	11.9	-12.5
6	5	5•	2.3	.7
6	-5	5	4.3	-4.2
-6	5	5	18.6	16.9
6	6	0	18.7	-18.0
6	-6	0	20.5	-20.5
6	6	1•	3.8	-.0
6	6	-1	5.2	-2.4
6	-6	1	28.1	-27.5
-6	6	1	14.0	15.4
6	6	2•	3.2	3.2
6	6	-2	16.4	-15.3
6	-6	2•	2.9	-2.1
-6	6	2•	2.5	-.9
6	6	3•	2.5	2.9
6	6	-3	21.7	-21.0
6	-6	3	29.8	-31.0
-6	6	3	4.6	-3.6
6	6	4•	1.7	6.3
6	6	-4	23.2	-24.0
6	-6	4	8.4	-8.9
-6	6	4	11.6	10.9
6	6	-5	17.1	-18.0
6	-6	5	5.4	-5.8
-6	6	5	13.4	13.7
6	7	0	13.4	-12.9
6	-7	0	6.9	5.9
6	7	1	15.9	16.8
6	7	-1	6.6	5.5
6	-7	1	25.5	-26.9
-6	7	1	9.7	9.0
6	7	2	11.8	13.4
6	7	-2	17.9	-18.6
6	-7	2	12.2	-13.3
-6	7	2	30.5	31.6
6	7	3	5.1	5.6
6	7	-3	29.6	-29.4
6	-7	3	22.5	-23.3
-6	7	3	34.8	35.8
6	7	-4•	2.9	5.1
6	-7	4	12.0	-12.9
-6	7	4	28.4	29.4
6	7	-5	14.1	-14.9
6	-7	5	4.2	4.3
-6	7	5	22.2	21.2
6	8	0•	4.9	6.2
6	-8	0•	4.6	2.5
6	8	1	18.0	20.2
6	8	-1	15.4	15.2
6	-8	1	23.7	22.9
-6	8	1•	3.5	5.8
6	8	2	9.4	8.9
6	8	-2	19.5	19.3
6	-8	2	9.1	9.5
-6	8	2	33.1	33.6
6	8	3	8.7	8.6
6	8	-3	13.7	-12.2

TABLE I (*continued*).

h	*k*	*l*	F_o	F_c
6	-8	3	5.3	-3.9
-6	8	3	5.4	-5.9
6	8	-4	12.3	13.3
6	-8	4•	3.0	-3.5
-6	8	4	21.9	22.2
6	8	-5•	2.7	-2.6
6	-8	5•	2.2	-3.4
-6	8	5	15.9	16.3
6	9	0	17.3	19.2
6	-9	0	7.9	7.6
6	9	1	8.1	7.5
6	9	-1	17.5	18.6
6	-9	1	36.8	37.1
-6	9	1	40.2	43.1
6	9	2	6.8	7.0
6	9	-2	21.8	24.4
6	-9	2	21.0	22.7
-6	9	2	26.8	29.0
6	9	-3	5.7	7.1
6	-9	3•	2.8	1.0
-6	9	3	17.0	-18.0
6	9	-4•	3.0	1.0
6	-9	4•	2.9	4.9
-6	9	4	10.5	11.6
6	9	-5•	2.8	-3.2
6	-9	5•	2.0	1.4
-6	9	5	8.1	-6.8
6	10	0•	4.5	4.9
6	-10	0•	4.9	5.2
6	10	1•	3.1	-1.2
6	10	-1	8.3	7.8
6	-10	1	17.6	17.2
-6	10	1	14.5	13.4
6	10	2•	1.9	3.0
6	10	-2•	2.9	3.6
6	-10	2•	3.0	4.5
-6	10	2	13.5	12.6
6	10	-3	9.6	9.0
6	-10	3	9.5	8.1
-6	10	3•	2.9	4.2
6	10	-4	14.8	15.1
6	-10	4	10.1	10.0
-6	10	4	5.3	2.7
6	10	-5	5.8	6.1
-6	10	5•	2.7	-4.3
6	11	0•	3.9	-4.2
6	-11	0	13.0	-13.7
6	11	1•	2.5	-3.9
6	11	-1•	3.6	-.3
6	-11	1	23.6	23.9
-6	11	1	9.9	-10.1
6	11	-2	7.5	8.1
6	-11	2	6.7	6.8
-6	11	2•	3.0	4.0
6	11	-3	6.6	6.5
6	-11	3	8.2	9.4
-6	11	3	16.0	-16.2
6	11	-4	15.3	16.7
6	-11	4	11.6	13.0
-6	11	4	7.4	-6.9
6	11	-5	11.7	13.9
-6	11	5•	2.5	1.2
6	12	0•	3.1	.7
6	-12	0	10.0	-9.1
6	12	-1•	2.7	-3.4
6	-12	1	14.4	12.4
-6	12	1•	3.7	.9
6	12	-2•	2.6	2.4
6	-12	2•	2.8	1.3
-6	12	2	10.0	-10.6
6	12	-3•	2.5	3.9
6	-12	3•	2.5	-.4
-6	12	3	18.9	-20.7
6	12	-4	5.3	-5.4
6	-12	4	10.1	11.4
-6	12	4	13.4	-14.2
6	12	-5	4.2	4.8
-6	12	5	12.1	-14.0
6	-13	0	12.4	-11.6
6	13	-1•	1.9	-3.4
6	-13	1	13.1	-12.3
-6	13	1	10.3	-10.5
6	13	-2	9.2	-10.8
6	-13	2•	2.7	-3.4
-6	13	2	15.0	-16.0
6	13	-3•	2.0	-2.0
6	-13	3•	2.3	-3.2
-6	13	3•	2.5	-5.2
6	13	-4•	2.1	-4.1
6	-13	4•	1.0	3.8
-6	13	4	12.5	-13.3
6	13	-5•	1.1	.5
6	-14	0	12.3	-12.9
6	-14	1	12.1	-12.1
-6	14	1	17.3	-19.6
6	-14	2	7.1	-8.2
-6	14	2	7.4	-7.7
6	-14	3•	1.8	-6.4
-6	14	3•	2.2	-1.4
6	-15	0•	3.6	-5.4
6	-15	1	8.3	-9.3
-6	15	1•	3.0	-3.1
-6	15	2•	2.1	-.1
6	-16	0•	2.2	2.2
7	0	0	21.8	-21.6
7	0	1	9.0	-9.9
7	0	-1	12.8	14.3
7	0	2•	3.0	-2.0
7	0	-2	5.9	4.9
7	0	3	11.8	-11.6
7	0	-3	9.0	10.4
7	0	4	4.1	-3.5
7	0	-4	12.8	13.1
7	0	5•	1.5	-.6
7	0	-5	12.3	-12.4
7	1	0•	4.3	3.8
7	-1	0•	4.3	-1.0
7	1	1•	3.6	3.0
7	1	-1	13.2	11.2
7	-1	1	12.9	-12.2
-7	1	1•	3.0	-1.6
7	1	2•	3.0	-2.6
7	1	-2	9.0	9.0
7	-1	2•	3.0	1.3
-7	1	2	20.8	-21.1
7	1	3•	3.0	-.4
7	1	-3	4.9	3.5
7	-1	3	6.1	-6.6
-7	1	3	16.0	-16.2
7	1	4•	2.8	-.4
7	1	-4	4.3	3.1
7	-1	4	8.1	-8.0
-7	1	4	7.4	-6.8
7	1	-5	4.5	-4.3
7	-1	5•	1.8	-4.2
-7	1	5	5.6	3.4
7	2	0	7.5	7.6
7	-2	0	9.7	9.6
7	2	1	11.0	-11.1
7	2	-1	5.4	6.3
7	-2	1	12.4	10.1
-7	2	1	8.2	-8.0
7	2	2	9.6	8.5
7	2	-2	22.2	-23.6
7	-2	2•	3.0	-3.9
-7	2	2	13.6	14.5
7	2	3	8.9	8.3
7	2	-3	10.0	8.5
7	-2	3•	2.8	-4.6
-7	2	3	13.5	-13.6
7	2	4•	2.6	-1.0
7	2	-4	8.0	5.1
7	-2	4•	3.0	-3.2
-7	2	4	8.1	-7.5
7	2	-5	16.5	16.3
7	-2	5	6.1	-6.8
-7	2	5	5.1	-4.8
7	3	0	10.2	-9.6
7	-3	0	6.8	-7.1
7	3	1	9.7	-10.5
7	3	-1	9.5	7.6
7	-3	1•	3.5	1.6
-7	3	1	13.7	13.2
7	3	2	9.1	9.3
7	3	-2	11.7	-10.9
7	-3	2•	3.0	4.4
-7	3	2	10.8	10.7
7	3	3•	2.8	1.0
7	3	-3	19.2	18.8
7	-3	3	5.2	-5.0
-7	3	3•	2.1	-.2
7	3	4•	2.3	.3
7	3	-4	18.7	17.0
7	-3	4•	3.1	1.6
-7	3	4	17.2	16.1
7	3	-5•	2.1	2.6
7	-3	5•	2.0	-3.6
-7	3	5	18.7	-18.7
7	4	0•	4.8	4.0
7	-4	0•	4.2	4.5
7	4	1•	4.8	1.4
7	4	-1	9.6	9.6
7	-4	1•	3.5	-.9
-7	4	1	5.1	-5.8
7	4	2•	3.1	2.5
7	4	-2•	2.7	-1.3
7	-4	2	9.0	8.4
-7	4	2	12.6	-12.7
7	4	3•	2.7	1.1
7	4	-3	6.7	-5.8
7	-4	3•	3.0	.9
-7	4	3	4.8	4.3
7	4	4•	1.9	.4
7	4	-4	4.9	4.0
7	-4	4•	3.1	-.1
-7	4	4	9.4	-7.8
7	4	-5	11.9	-10.7
7	-4	5•	2.0	1.6
-7	4	5•	2.2	-1.9
7	5	0	9.0	7.9
7	-5	0	11.1	10.9
7	5	1•	3.8	-2.5
7	5	-1•	3.6	-2.0
7	-5	1	8.9	9.2
-7	5	1	7.4	-5.7
7	5	2•	3.0	5.6
7	5	-2	10.5	-10.7
7	-5	2•	3.0	.3
-7	5	2•	2.5	3.5
7	5	3•	2.3	4.2
7	5	-3	5.1	-4.1
7	-5	3	9.7	10.1
-7	5	3	10.5	-9.0
7	5	-4	5.0	-4.4
7	-5	4•	2.9	4.4
-7	5	4	17.4	-17.3
7	5	-5•	2.5	-.4
7	-5	5•	2.0	3.1
-7	5	5	10.3	10.4
7	6	0	7.7	-6.4
7	-6	0•	4.5	1.1
7	6	1	5.9	-7.5
7	6	-1	7.1	5.9
7	-6	1	12.7	12.3
-7	6	1	5.0	4.2
7	6	2	6.8	7.8
7	6	-2	10.9	-12.2
7	-6	2•	3.0	2.5
-7	6	2	4.0	2.8
7	6	3•	2.0	-2.0
7	6	-3•	2.8	-.1
7	-6	3	12.3	11.3
-7	6	3	6.2	5.3
7	6	-4	11.6	11.2
7	-6	4	10.0	10.0
-7	6	4	12.5	11.7
7	6	-5	8.9	-9.7
7	-6	5	4.0	5.1
-7	6	5•	2.6	2.3
7	7	0•	4.8	-7.2
7	-7	0•	4.6	-1.6
7	7	1•	3.7	.1
7	7	-1	8.2	8.7
7	-7	1	5.8	4.1
-7	7	1	16.1	-17.0
7	7	2•	2.8	1.1
7	7	-2•	3.0	-1.8
7	-7	2•	3.0	-1.1
-7	7	2•	2.8	-1.0
7	7	-3	16.1	-16.0
7	-7	3	5.7	6.4
-7	7	3	21.8	22.8
7	7	-4•	3.0	4.2
7	-7	4	4.1	4.9
-7	7	4•	2.9	-4.6
7	7	-5	15.2	-15.4
-7	7	5	8.1	8.6
7	8	0•	4.6	3.6
7	-8	0•	4.8	5.0
7	8	1•	3.2	-.6
7	8	-1•	3.8	-.3
7	-8	1	11.5	-12.0
-7	8	1	13.7	-14.2
7	8	2•	2.3	.7
7	8	-2	6.1	-5.5
7	-8	2	15.3	-17.2
-7	8	2•	2.9	3.2
7	8	-3	6.9	-7.2
7	-8	3	4.8	4.7
-7	8	3•	2.8	-2.3
7	8	-4•	3.1	-4.1
7	-8	4•	2.8	-1.2
-7	8	4	20.0	-21.5
7	8	-5	6.0	-6.2
-7	8	5	9.8	10.7
7	9	0•	4.5	2.1
7	9	1	6.6	-7.3
7	9	-1	10.7	10.6
7	-9	1•	3.8	-.3
-7	9	1	12.3	-12.7
7	9	-2	7.1	-8.8
7	-9	2	14.8	-16.6
-7	9	2	6.4	7.0
7	9	-3	7.7	7.2
7	-9	3•	2.7	-3.1
-7	9	3•	2.3	3.8
7	9	-4	6.5	7.3
7	-9	4•	2.6	-2.1
-7	9	4•	3.2	-1.2
7	9	-5	9.6	-10.3
-7	9	5•	2.8	-.5
7	10	0•	3.9	-2.4
7	-10	0•	4.9	4.2
7	10	1•	2.5	-2.8
7	10	-1	9.1	10.4
7	-10	1•	3.8	-4.8
-7	10	1	9.3	-9.1
7	10	-2•	2.7	1.3
7	-10	2•	2.8	-4.5
-7	10	2•	3.0	-5.5
7	10	-3•	2.8	5.0
7	-10	3	5.3	-4.4
-7	10	3	12.2	12.3
7	10	-4	7.5	8.7
7	-10	4	6.7	-7.3
-7	10	4•	3.2	1.5
7	10	-5	5.1	-5.5
-7	10	5•	2.8	-2.7
7	11	0•	3.1	3.6
7	-11	0	12.8	12.9
7	11	-1•	2.8	-1.4
7	-11	1	8.7	-7.6
-7	11	1•	3.8	-1.6
7	11	-2•	2.5	-2.2
7	-11	2	5.2	-5.4
-7	11	2•	3.0	.6
7	11	-3	5.8	6.2
7	-11	3•	2.8	-1.9
-7	11	3•	2.9	4.8
7	11	-4	5.1	4.9
7	-11	4	6.5	-8.2
-7	11	4	11.7	-11.6
7	11	-5	7.3	8.0
-7	11	5•	2.5	-2.6
7	-12	0•	4.7	4.0
7	12	-1•	2.1	1.2
7	-12	1•	3.8	1.6
-7	12	1•	3.6	-2.2
7	12	-2	5.1	-6.4
7	-12	2	4.7	-5.5
-7	12	2	7.1	7.8
7	12	-3	6.8	7.5
7	-12	3•	2.3	.6
-7	12	3•	2.8	2.8
7	12	-4•	2.3	3.0
-7	12	4•	3.2	-.4
7	12	-5•	1.8	1.0
-7	12	5	4.4	-3.0
7	-13	0•	4.5	4.0
7	-13	1	5.4	4.0
-7	13	1•	3.3	4.0
7	-13	2	6.9	7.7
-7	13	2	7.5	-7.8
7	-13	3	5.0	5.4
-7	13	3•	2.5	-.6
-7	13	4	4.8	4.2
7	-14	0	11.5	13.6
7	-14	1	8.3	9.6
-7	14	1•	3.5	1.3
7	-14	2	4.9	5.2
-7	14	2•	2.5	.4
-7	14	3	4.3	5.2
7	-15	0•	3.4	-1.9
7	-15	1•	2.2	.1
-7	15	1•	2.6	-5.4
-7	15	2•	1.9	5.5
8	0	0	23.3	-21.0
8	0	1•	3.8	3.2
8	0	-1	24.8	-23.7
8	0	2	28.6	-31.2
8	0	-2	32.1	32.3
8	0	3	11.5	-12.6
8	0	-3	16.8	-17.3
8	0	4	5.5	-5.2
8	0	-4	20.1	19.3
8	0	-5	33.7	35.4
8	1	0	30.5	-28.8
8	-1	0	8.3	-4.6
8	1	1•	3.8	-6.0
8	1	-1	43.1	-49.4
8	-1	1	12.1	11.5
-8	1	1	7.0	6.5
8	1	2	20.9	-21.0
8	1	-2	27.2	28.4
8	-1	2	18.7	-20.0
-8	1	2	29.7	29.1
8	1	3	6.0	-5.4
8	1	-3	26.0	-27.3
8	-1	3	10.9	-11.9
-8	1	3	15.7	14.3
8	1	4•	2.1	-.6
8	1	-4	15.9	-14.5
8	-1	4	5.3	-6.2
-8	1	4	11.7	11.4
8	1	-5	28.0	27.3
-8	1	5	13.6	13.5
8	2	0	19.8	-18.9
8	-2	0	8.1	5.4
8	2	1•	3.8	-2.8
8	2	-1	34.0	-35.4
8	-2	1	22.8	21.9
-8	2	1	10.8	10.5
8	2	2•	3.1	-2.7
8	2	-2	12.4	-11.0
8	-2	2•	3.0	-4.7
-8	2	2	30.4	29.4
8	2	3•	2.5	-4.0
8	2	-3	37.7	-37.8
8	-2	3•	2.8	-.2
-8	2	3	29.5	29.6
8	2	-4	26.0	-23.5
8	-2	4•	2.7	-.4
-8	2	4•	2.4	1.1
8	2	-5	6.5	-5.8
-8	2	5	20.5	19.6
8	3	0	13.4	-11.5
8	-3	0•	4.6	4.0
8	3	1	9.8	10.0
8	3	-1	8.2	-7.5
8	-3	1	30.7	32.9
-8	3	1	23.2	23.1
8	3	2	6.9	6.9
8	3	-2•	2.8	-2.4
8	-3	2	7.9	7.5
-8	3	2	21.3	20.8
8	3	3•	2.5	-1.5
8	3	-3	40.7	-43.3
8	-3	3•	2.9	2.7
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8	3	-4	13.1	-13.1
8	-3	4	8.3	8.3
-8	3	4	9.8	8.2
8	3	-5	4.7	4.3
-8	3	5	16.9	16.9
8	4	0•	4.9	.9
8	-4	0•	4.6	3.1
8	4	1	10.3	10.0
8	4	-1	5.5	3.6
8	-4	1	23.1	24.4
-8	4	1	36.3	37.9
8	4	2	9.7	10.3
8	4	-2	14.9	14.7
8	-4	2	15.7	16.3
-8	4	2	21.3	20.6
8	4	3•	2.3	3.8
8	4	-3	7.7	-7.0
8	-4	3•	2.9	-2.1
-8	4	3•	2.5	1.1
8	4	-4	17.7	-15.3
8	-4	4	12.2	13.1
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8	4	-5•	2.5	3.8
-8	4	5	5.7	-4.5
8	5	0	8.0	7.1
8	-5	0	8.3	8.2
8	5	1	9.4	10.0
8	5	-1	16.0	15.8
8	-5	1	17.1	15.3
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8	5	2	12.6	13.4
8	5	-2•	3.0	-1.1
8	-5	2	13.8	13.5
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8	5	3•	1.9	3.3
8	5	-3	7.8	8.5
8	-5	3•	2.9	4.3
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8	5	-4	10.4	-10.2
8	-5	4	15.2	15.7
-8	5	4	21.8	-21.3
8	5	-5	10.4	-10.1
-8	5	5	3.8	-5.7
8	6	0•	4.8	2.5
8	-6	0	12.7	-12.5
8	6	1	14.5	16.0
8	6	-1	17.8	19.6
8	-6	1	19.3	19.0
-8	6	1	36.2	-39.8
8	6	2	7.8	8.1
8	6	-2•	3.0	5.3
8	-6	2	7.5	7.3
-8	6	2	5.2	5.9
8	6	-3•	2.3	1.0
8	-6	3	5.2	6.0
-8	6	3	43.6	-45.8
8	6	-4	11.8	10.6
8	-6	4	13.4	14.6
-8	6	4	33.5	-34.6
8	6	-5•	2.7	3.7
-8	6	5•	2.6	3.9
8	7	0•	4.5	5.7
8	-7	0	20.3	-19.5
8	7	1	9.6	10.2
8	7	-1	11.5	10.7
8	-7	1•	3.8	-1.0
-8	7	1	28.3	-29.3
8	7	2•	2.2	-3.7
8	7	-2	13.1	20.9
8	-7	2	13.0	-13.8
-8	7	2•	2.9	5.7
8	7	-3	12.1	12.9
8	-7	3	5.4	-5.5
-8	7	3	36.8	-38.5
8	7	-4	13.7	14.8
8	-7	4	7.0	6.9
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8	7	-5	12.3	13.7
-8	7	5	5.3	2.9
8	8	0•	4.4	1.0
8	-8	0	17.9	-17.1
8	8	1•	2.7	-2.1
8	8	-1•	3.7	5.6
8	-8	1	16.5	-15.4
-8	8	1	36.6	-40.6
8	8	-2	13.1	14.4
8	-8	2	25.6	-29.5
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8	8	-3	10.9	11.4
8	-8	3	6.9	-7.2
-8	8	3•	2.8	1.1
8	8	-4	6.2	5.6
8	-8	4•	2.6	-2.8
-8	8	4•	3.0	-2.0
8	8	-5	8.4	7.2
-8	8	5	12.7	11.5
8	9	0	10.1	-11.1
8	-9	0	11.4	-12.8
8	9	1	4.0	-5.6
8	9	-1	8.2	-8.2
8	-9	1	5.9	3.9
-8	9	1	25.3	-26.0
8	9	-2•	2.7	-.7
8	-9	2	22.3	-23.3
-8	9	2	17.8	18.4
8	9	-3•	2.8	-4.5
8	-9	3	5.5	-4.6
-8	9	3•	2.9	-1.5
8	9	-4	8.8	8.6
8	-9	4	5.4	-5.9
-8	9	4•	3.2	-3.1
8	9	-5	6.3	6.1
-8	9	5	18.6	19.8
8	10	0	8.4	-9.1
8	-10	0•	4.9	4.3
8	10	-1	12.5	-14.8
8	-10	1	9.3	9.0
-8	10	1	9.1	10.3
8	10	-2•	2.4	-2.6
8	-10	2	13.8	-14.9
-8	10	2	12.0	12.3
8	10	-3	8.7	-10.3
8	-10	3	5.0	-5.1
-8	10	3•	2.8	5.2
8	10	-4•	2.8	1.8
-8	10	4	9.8	9.7
8	10	-5	7.3	7.4
-8	10	5	6.3	5.9
8	-11	0•	4.7	3.5
8	11	-1	7.2	-7.2
8	-11	1•	3.7	3.8
-8	11	1	11.9	12.4
8	11	-2	3.9	-3.5
8	-11	2•	2.7	-2.4
-8	11	2	10.6	10.9
8	11	-3	6.8	-6.8
8	-11	3•	2.1	-1.9
-8	11	3	22.7	24.2
8	11	-4	10.1	-12.3
-8	11	4	9.8	10.5
8	11	-5•	2.0	-2.4
-8	11	5	6.1	7.3
8	-12	0	11.3	11.1
8	-12	1	12.3	11.3
-8	12	1	9.6	9.1
8	-12	2	4.2	4.8
-8	12	2	10.7	11.4
8	-12	3•	1.9	3.6
-8	12	3	12.7	13.9
-8	12	4	5.3	4.9
-8	12	5	8.3	8.9
8	-13	0	12.2	11.8
8	-13	1	13.7	14.4
-8	13	1	12.3	13.0
8	-13	2	10.0	11.4
-8	13	2	5.5	5.4
-8	13	3•	2.4	-3.0
-8	13	4	3.5	-4.5
8	-14	0•	3.7	3.6
8	-14	1	6.2	5.6
-8	14	1•	3.2	3.9
-8	14	2•	2.3	.0
-8	14	3	4.3	-4.5
8	-15	0•	2.7	-1.6
9	0	0•	4.9	1.8
9	0	1•	3.8	7.6
9	0	-1•	3.6	-1.6
9	0	2•	2.9	1.4
9	0	-2	15.4	16.0
9	0	3•	2.4	3.5
9	0	-3•	3.3	2.6
9	0	-4•	2.8	1.5
9	0	-5	10.6	9.3
9	1	0•	4.9	.6
9	-1	0	11.3	-11.0
9	1	1•	3.7	5.2
9	1	-1•	3.7	.5
9	-1	1•	3.9	-.6
-9	1	1•	3.6	3.7
9	1	2	7.9	7.3
9	1	-2	5.3	-5.6
9	-1	2•	3.1	.6
-9	1	2	7.4	6.7
9	1	3•	2.3	3.4
9	1	-3	4.7	-6.1
9	-1	3•	2.4	-2.3
-9	1	3	4.7	-4.4
9	1	-4•	2.8	1.4
-9	1	4	14.9	15.0
9	1	-5	16.9	16.3
-9	1	5•	2.4	.8
9	2	0	13.2	-12.9
9	-2	0•	4.8	-3.0
9	2	1•	3.7	4.2
9	2	-1	6.1	6.0
9	-2	1	6.1	-5.4
-9	2	1•	3.6	-4.3
9	2	2•	2.8	3.7
9	2	-2•	2.9	-1.2
9	-2	2•	3.0	1.6
-9	2	2	8.1	-8.9
9	2	3•	2.0	-2.1
9	2	-3	12.9	-13.5
9	-2	3•	2.5	-3.5
-9	2	3•	2.7	-.6
9	2	-4•	2.9	5.1
9	-2	4•	1.7	1.1
-9	2	4•	2.7	1.9
9	2	-5•	2.5	2.5
-9	2	5•	2.4	-.1
9	3	0•	4.9	-5.6
9	-3	0•	4.8	3.2
9	3	1•	3.8	5.1
9	3	-1	4.9	4.6
9	-3	1•	3.8	-3.1
-9	3	1•	3.6	-.4
9	3	2•	2.6	-.2
9	3	-2	5.2	6.4
9	-3	2•	3.0	-4.8
-9	3	2	4.6	4.3
9	3	-3	11.8	-10.9
9	-3	3•	2.7	-2.8
-9	3	3	4.2	-3.3
9	3	-4•	2.9	-3.9
-9	3	4•	2.8	-2.8
9	3	-5	8.4	-7.6
-9	3	5•	2.5	.0
9	4	0•	4.8	-1.6
9	-4	0•	4.8	-5.4
9	4	1•	3.5	-2.2
9	4	-1	8.3	8.9
9	-4	1•	4.0	-2.6
-9	4	1•	3.6	1.3
9	4	2•	2.5	3.7
9	4	-2	7.5	-7.8
9	-4	2	6.2	-5.7
-9	4	2	4.7	4.2
9	4	-3	8.6	-8.7
9	-4	3	4.6	-5.7
-9	4	3	6.2	5.0
9	4	-4•	3.0	.5
9	-4	4•	1.8	-4.5
-9	4	4	12.0	11.6
9	4	-5	5.8	-5.7
-9	4	5	10.1	-9.8
9	5	0	9.4	-9.1
9	-5	0•	4.9	-1.0
9	5	1•	3.3	-3.3
9	5	-1	9.5	9.8
9	-5	1	6.6	-6.7
-9	5	1•	3.7	-2.0
9	5	2•	2.3	4.5
9	5	-2•	3.0	-5.3
9	-5	2•	2.9	-3.8
-9	5	2	9.5	-9.1
9	5	-3•	2.9	-3.2
9	-5	3	4.4	-3.9
-9	5	3	9.2	10.3
9	5	-4	10.3	11.5
-9	5	4	10.0	-8.8
9	5	-5	10.6	-10.5
-9	5	5	9.4	-9.6
9	6	0•	4.6	-5.1
9	-6	0	12.7	13.0
9	6	1•	3.0	-.9
9	6	-1•	3.6	5.9
9	-6	1•	3.8	-1.6
-9	6	1•	3.7	4.1
9	6	2•	1.7	.5
9	6	-2•	3.0	1.5
9	-6	2•	2.9	-1.5
-9	6	2	6.5	-6.9
9	6	-3	6.5	-7.4
9	-6	3•	2.5	2.7
-9	6	3	5.1	-2.9
9	6	-4	7.5	7.7
-9	6	4	18.5	-19.4
9	6	-5	6.9	-6.7
-9	6	5•	2.6	-.5
9	7	0•	4.1	1.6
9	-7	0	11.0	10.5
9	7	1•	2.5	-1.6
9	7	-1•	3.6	3.2
9	-7	1	8.5	8.9
-9	7	1•	3.8	.4
9	7	-2•	2.9	.2
9	-7	2•	2.9	3.3
-9	7	2•	3.0	1.1
9	7	-3•	2.8	-.9
9	-7	3	6.1	5.8
-9	7	3	11.6	11.5
9	7	-4•	3.0	2.1
9	-7	4•	1.6	.1
-9	7	4	5.5	4.5
9	7	-5•	2.7	.3
-9	7	5•	2.8	-2.3
9	8	0•	3.6	-2.1
9	-8	0•	4.9	3.7
9	8	1•	1.6	-1.0
9	8	-1	6.4	6.4
9	-8	1•	3.8	-.0
-9	8	1•	3.8	3.3
9	8	-2•	2.7	1.4
9	-8	2	7.9	8.6
-9	8	2	8.1	-7.9
9	8	-3	5.0	4.4
9	-8	3	6.9	7.6
-9	8	3	7.4	8.0
9	8	-4	9.8	11.2
-9	8	4•	3.2	3.4
9	8	-5•	2.7	1.5
-9	8	5•	3.0	-1.1
9	9	0•	2.9	-4.6
9	-9	0	7.0	7.4
9	9	-1•	2.8	2.4
9	-9	1•	3.8	-2.4
-9	9	1•	4.1	-1.8
9	9	-2	4.9	4.7
9	-9	2	4.7	4.7
-9	9	2	6.6	-6.4
9	9	-3•	2.6	-3.4
9	-9	3	7.1	7.4
-9	9	3•	2.9	-1.0
9	9	-4	7.6	8.6
-9	9	4	8.4	-7.6
9	9	-5	6.1	6.7
-9	9	5•	2.6	-.8
9	-10	0•	4.7	1.3
9	10	-1•	2.2	-2.5
9	-10	1•	3.4	-1.5
-9	10	1•	3.8	-4.9
9	10	-2•	2.2	-.4
9	-10	2•	2.7	-1.0
-9	10	2•	3.0	1.7
9	10	-3•	2.2	-3.4
9	-10	3	4.1	4.0
-9	10	3•	2.8	1.5
9	10	-4•	2.5	.4
-9	10	4	4.9	4.6
9	10	-5	8.0	8.1
-9	10	5•	2.6	-.6
9	-11	0•	4.7	-2.9
9	-11	1	5.4	-5.5
-9	11	1•	3.7	-.9
9	11	-2•	1.2	-4.5
9	-11	2•	2.6	-.4
-9	11	2	6.6	-7.4
9	-11	3•	1.4	-.9
-9	11	3•	2.7	-1.3
9	11	-4•	1.6	1.1
-9	11	4	7.2	7.5
-9	11	5•	2.3	-1.2
9	-12	0•	4.3	2.5
9	-12	1	8.3	-7.8
-9	12	1•	3.4	-6.3
9	-12	2	5.4	-6.0
-9	12	2•	2.9	-4.3
-9	12	3	6.2	7.7
-9	12	4	4.2	-4.4
-9	12	5•	1.6	-3.0
9	-13	0•	3.9	-1.3
9	-13	1	10.2	-10.3
-9	13	1•	3.1	-3.2
-9	13	2•	2.5	1.2
-9	13	3•	2.3	3.1
-9	13	4•	1.9	-2.1
9	-14	0•	3.2	4.6
9	-14	1•	1.6	-1.7
-9	14	1•	2.6	2.3
-9	14	2	4.8	-5.5
10	0	0•	4.9	-5.0
10	0	1•	3.7	5.9
10	0	-1	20.4	-21.1
10	0	2•	2.5	-2.6
10	0	-2	8.6	-8.7
10	0	-3	13.9	-13.9
10	0	-4	20.8	-20.8
10	0	-5	11.3	-11.3
10	1	0	13.0	11.4
10	-1	0	21.5	21.3
10	1	1	12.8	13.2
10	1	-1	7.1	-7.2
10	-1	1•	3.8	.9
-10	1	1	20.7	-21.7
10	1	2	5.5	6.0
10	1	-2•	3.0	.4
10	-1	2	13.0	-14.3
-10	1	2	7.5	-7.0
10	1	-3	11.3	-11.3
10	-1	3•	1.9	.6
-10	1	3	19.0	-20.6
10	1	-4	21.7	-20.6
-10	1	4	11.1	-10.6
10	1	-5	23.1	-23.7
-10	1	5•	2.6	2.0
10	2	0	20.9	21.9
10	-2	0	20.8	-20.3
10	2	1	12.2	14.2
10	2	-1•	3.8	-.9
10	-2	1•	3.8	-2.4
-10	2	1	14.9	-13.8
10	2	2•	2.3	3.6
10	2	-2	17.2	18.3
10	-2	2	15.9	-17.1
-10	2	2	7.4	-6.9
10	2	-3•	2.8	1.1
10	-2	3	7.1	-7.5
-10	2	3	9.3	-8.5
10	2	-4	6.5	-5.4
-10	2	4	13.3	-12.8
10	2	-5•	2.7	1.1
-10	2	5•	2.6	3.1
10	3	0	20.2	20.8
10	-3	0	8.9	-6.4
10	3	1	5.9	6.0
10	3	-1•	4.0	-.3
10	-3	1•	3.7	-4.1
-10	3	1	21.6	-21.8
10	3	2•	2.1	.6
10	3	-2	26.4	29.5
10	-3	2	14.4	-15.4
-10	3	2•	3.0	-1.2
10	3	-3	22.2	22.8
10	-3	3	6.8	-6.9
-10	3	3	15.3	-16.0
10	3	-4	6.7	-6.4
-10	3	4	14.1	-13.3
10	3	-5	19.0	18.6
-10	3	5	20.2	20.6
10	4	0	10.5	9.5
10	-4	0•	4.9	5.4
10	4	1•	3.1	1.0
10	4	-1•	3.9	.3
10	-4	1•	3.8	-.7
-10	4	1	17.2	-18.0
10	4	2•	1.6	-.4
10	4	-2	12.8	13.9
10	-4	2	12.5	-13.7
-10	4	2	21.0	22.0
10	4	-3	19.6	21.4
10	-4	3	5.0	-5.0
-10	4	3	20.4	20.8
10	4	-4•	3.1	-1.6
-10	4	4	10.2	-10.5
10	4	-5	12.0	12.0
-10	4	5	32.3	35.9
10	5	0•	4.3	-1.9
10	-5	0	21.9	22.7
10	5	1•	2.5	1.2
10	5	-1•	3.8	-1.9
10	-5	1•	3.8	.9
-10	5	1•	3.8	-1.3
10	5	-2	5.9	5.4
10	-5	2	8.8	-8.7
-10	5	2	24.7	25.4
10	5	-3	6.3	5.3
10	-5	3•	2.0	-1.9
-10	5	3	29.3	31.0
10	5	-4•	3.1	3.3
-10	5	4	5.1	3.1
10	5	-5	18.9	19.3
-10	5	5	22.4	21.5
10	6	0	6.2	-6.4
10	-6	0	33.8	34.4
10	6	1•	2.1	-3.5
10	6	-1•	3.4	-4.5
10	-6	1	7.3	6.5
-10	6	1•	3.8	-1.9
10	6	-2	4.6	3.8
10	-6	2•	2.7	2.1
-10	6	2	20.3	21.0
10	6	-3•	2.9	4.8
10	-6	3	8.2	8.7
-10	6	3	31.0	33.8
10	6	-4•	3.0	-1.4
-10	6	4	7.0	-9.9
-10	6	5•	2.7	2.2
10	7	0	9.6	-10.3
10	-7	0	30.5	30.5
10	7	-1	5.5	-4.9
10	-7	1	17.1	17.0

TABLE I (*continued*).

h	*k*	*l*	F_o	F_c	*h*	*k*	*l*	F_o	F_c	*h*	*k*	*l*	F_o	F_c	*h*	*k*	*l*	F_o	F_c	*h*	*k*	*l*	F_o	F_c	*h*	*k*	*l*	F_o	F_c
-10	7	1•	3.8	-4.9	-11	1	1•	3.7	.3	11	-6	2	3.9	-4.5	12	1	-5	11.6	10.8	12	-8	0	12.1	13.4	13	5	-3•	1.7	1.4
10	7	-2	6.2	-6.7	11	1	2•	1.7	-2.7	-11	6	2	7.4	-7.6	-12	1	5	8.6	-7.4	12	-8	1	5.9	5.3	-13	5	3•	2.6	2.7
10	-7	2	7.0	6.8	11	1	-2•	3.0	1.9	11	6	-3•	2.7	-3.4	12	2	0•	3.6	2.1	-12	8	1•	3.3	6.0	13	5	-4•	1.9	-4.8
-10	7	2	14.8	16.1	11	-1	2•	2.3	1.9	-11	6	3•	2.5	.5	12	-2	0	10.2	10.7	-12	8	2	13.3	13.0	-13	5	4•	3.0	-2.8
10	7	-3•	2.7	-.3	-11	1	2	6.7	7.3	11	6	-4•	2.8	2.1	12	-2	0	10.2	10.7	-12	8	3	13.9	15.5	13	5	-5•	1.7	-.7
10	-7	3	14.5	15.8	11	1	-3	9.2	-9.9	-11	6	4•	3.5	-.5	12	2	-1	5.3	-5.4	-12	8	4	7.3	6.6	-13	5	5•	3.0	2.7
-10	7	3	5.1	4.5	-11	1	3	5.1	-5.0	11	6	-5	5.6	6.3	12	-2	1•	2.6	2.3	-12	8	5	8.4	8.1	13	-6	0•	3.4	.8
10	7	-4•	2.9	-3.7	11	1	-4•	3.2	-2.4	-11	6	5•	2.8	-2.2	-12	2	1•	3.4	-2.3	12	-9	0	10.2	11.2	-13	6	1•	3.0	.3
-10	7	4	19.1	-18.6	-11	1	4•	3.6	.9	11	-7	0•	4.7	1.1	12	2	-2	10.4	10.6	12	-9	1	5.4	8.3	-13	6	2•	2.5	-.4
10	7	-5•	2.6	-1.7	11	1	-5•	2.6	-1.8	11	7	-1•	2.3	2.9	-12	2	2	9.5	-9.9	-12	9	1	8.0	10.0	-13	6	3•	2.2	1.0
-10	7	5	4.9	-4.5	-11	1	5•	2.7	2.1	11	-7	1	5.4	-5.1	12	2	-3	13.0	12.9	-12	9	2	8.3	9.1	13	6	-4•	.8	-1.8
10	-8	0	9.9	10.6	11	2	0•	4.5	-1.5	-11	7	1•	3.6	-.1	-12	2	3	10.7	11.1	-12	9	3	9.6	11.0	-13	6	4•	3.2	3.2
10	8	-1	7.8	-8.3	11	-2	0•	4.7	-3.1	11	7	-2•	2.3	3.3	12	2	-4	10.4	10.1	-12	9	4•	2.7	2.9	-13	6	5	5.6	5.6
10	-8	1	9.3	9.5	11	2	1•	2.7	.8	11	-7	2	4.5	-5.0	-12	2	4	18.5	-19.8	-12	9	5•	2.1	.2	13	-7	0•	3.3	-3.3
-10	8	1•	3.7	-3.5	11	2	-1•	3.7	-3.0	-11	7	2•	3.0	-3.2	12	2	-5	13.5	13.4	12	-10	0	11.0	10.9	-13	7	1•	2.8	-.9
10	8	-2	8.8	-10.3	11	-2	1	5.2	5.1	11	7	-3•	2.4	-4.6	-12	2	5	9.3	-8.3	-12	10	1	7.3	7.3	-13	7	2•	2.6	-2.5
10	-8	2•	2.7	2.7	-11	2	1•	3.7	-.5	-11	7	3•	2.8	1.0	12	3	0•	3.4	-2.9	-12	10	2•	2.7	-3.5	-13	7	3•	2.5	-1.5
-10	8	2•	3.0	-4.5	11	2	-2	5.4	7.2	11	7	-4	6.4	7.6	12	-3	0	6.9	6.9	-12	10	3	10.5	12.4	-13	7	4•	2.6	2.2
10	8	-3	11.0	-13.2	11	-2	2•	2.3	2.9	-11	7	4	7.0	-7.1	12	3	-1	9.1	-10.2	-12	10	4•	2.4	-2.1	-13	7	5•	2.3	.8
-10	8	3	10.8	-11.7	-11	2	2	6.6	6.8	11	7	-5•	2.2	2.2	12	-3	1	5.4	-5.3	-12	11	1•	2.5	2.2	13	-8	0•	2.8	-2.5
10	8	-4•	2.6	-3.8	11	2	-3•	3.0	-1.4	-11	7	5•	2.8	-2.6	-12	3	1	5.7	-5.7	-12	11	2	7.6	-8.3	-13	8	1•	2.8	1.2
-10	8	4	7.7	-7.4	-11	2	3•	2.9	-4.3	11	-8	0•	4.5	2.8	12	3	-2•	2.7	-3.5	-12	11	3	5.1	5.0	-13	8	2•	2.4	-2.5
10	8	-5	4.8	-5.8	11	2	-4	10.4	-9.5	11	-8	1•	3.1	-2.1	-12	3	2	20.7	-22.3	-12	12	1•	1.6	-2.2	-13	8	3•	2.4	-2.4
-10	8	5	14.6	-15.9	-11	2	4	7.6	7.6	-11	8	1•	3.6	2.2	12	3	-3•	2.7	2.3	13	0	0•	3.1	-1.7	-13	8	4•	2.5	1.2
10	-9	0	8.9	-8.8	11	2	-5•	2.8	-.6	11	8	-2•	1.8	2.6	-12	3	3	5.2	5.5	13	0	-1	5.2	-4.8	-13	8	5•	2.2	-2.2
10	9	-1•	1.7	-7.4	-11	2	5•	2.6	-1.8	11	-8	2•	2.1	-3.4	12	3	-4•	2.7	2.0	13	0	-2	5.7	5.1	13	-9	0•	1.8	-4.1
10	-9	1•	3.6	-1.0	11	3	0•	4.2	-.7	11	8	-3	6.2	-7.4	-12	3	4	19.3	-19.2	13	0	-3•	2.9	-3.0	-13	9	1•	2.5	-.2
-10	9	1	13.3	-12.9	11	-3	0•	4.7	.1	-11	8	3•	2.8	2.3	12	3	-5•	2.6	2.8	13	0	-4•	2.8	-3.1	-13	9	2•	2.3	-.5
10	9	-2	4.3	-4.6	11	3	1•	2.5	.4	11	8	-4•	2.1	3.2	-12	3	5	19.7	-19.2	13	0	-5•	2.7	1.3	-13	9	3•	2.0	-3.3
10	-9	2	3.9	-3,0	11	3	-1•	3.7	-.8	-11	8	4•	3.0	3.7	12	4	0•	2.5	-2.5	13	1	0•	2.4	-.5	-13	9	4	5.5	5.4
-10	9	2	13.4	-13.1	11	-3	1	5.8	1.8	11	8	-5•	1.9	2.4	12	-4	0•	4.4	3.2	13	-1	0•	3.3	.6	-13	9	5•	1.5	.7
10	9	-3	9.0	-10.2	-11	3	1•	3.8	1.2	-11	8	5•	2.9	-.9	12	4	1•	.0	-6.9	13	1	-1	4.9	-5.2	-13	10	2•	2.1	-.3
-10	9	3	6.6	-6.5	11	3	-2•	2.9	3.5	11	-9	0•	4.3	2.1	12	4	-1	10.0	-11.6	-13	1	1•	2.7	-2.7	14	0	-1•	1.6	.7
10	9	-4	5.4	-6.7	11	-3	2•	2.3	4.0	11	-9	1•	3.0	-.3	12	-4	1	11.1	-13.1	13	1	-2	5.0	6.7	14	0	-2	6.9	-8.3
-10	9	4	10.4	-10.6	-11	3	2	4.2	-4.1	-11	9	1•	4.0	3.3	-12	4	1	13.0	-13.9	-13	1	2•	2.6	.1	14	0	-3	4.7	5.5
10	9	-5	6.0	-5.0	11	3	-3	4.9	4.2	-11	9	2•	2.7	-2.3	-12	4	2	24.1	-25.3	13	1	-3•	2.5	1.2	14	0	-4	6.2	8.3
-10	9	5	14.2	-14.8	-11	3	3•	2.9	-3.7	-11	9	3•	2.8	-.8	12	4	-3	5.1	-5.2	-13	1	3•	2.8	-1.4	14	0	-5•	2.3	-1.9
10	-10	0	9.0	-9.2	11	3	-4•	3.0	-3.0	-11	9	4•	2.9	4.8	-12	4	3•	2.8	2.2	13	1	-4•	2.9	-3.1	14	1	-2	9.1	-11.5
10	-10	1•	3.3	-1.6	-11	3	4•	3.0	.4	-11	9	5•	2.5	-3.4	12	4	-4	5.7	-6.7	-13	1	4•	3.5	-2.1	-14	1	2	4.6	-5.1
-10	10	1	14.4	-15.4	11	3	-5	7.1	6.3	11	-10	0	6.3	7.0	-12	4	4	20.0	-19.5	13	1	-5	5.5	6.1	14	1	-3•	2.0	-.2
10	-10	2	8.1	-8.4	-11	3	5•	2.7	-1.1	11	-10	1•	2.5	-1.1	12	4	-5•	2.6	.3	-13	1	5•	2.8	-1.5	-14	1	3	8.5	10.3
-10	10	2	12.7	-13.3	11	4	0•	3.9	-4.8	-11	10	1•	3.4	4.1	-12	4	5	17.8	-16.6	13	-2	0•	3.5	1.9	14	1	-4•	2.3	1.2
10	10	-3•	1.5	-1.7	11	-4	0•	4.7	3.0	-11	10	2•	2.9	-3.1	12	-5	0•	4.3	-1.4	13	2	-1•	2.4	-2.2	-14	1	4	11.3	11.7
-10	10	3	10.6	-10.7	11	4	1•	2.1	2.5	-11	10	3•	2.6	3.2	12	5	-1	6.9	-8.0	-13	2	1•	2.8	-2.4	14	1	-5	6.4	-6.3
-10	10	4	12.0	-13.0	11	4	-1•	3.6	-.5	-11	10	4•	2.7	-1.6	12	-5	1	12.1	-16.1	13	2	-2	3.9	4.1	-14	1	5•	2.3	-2.2
-10	10	5•	2.5	-2.2	11	-4	1•	3.5	.9	-11	10	5	3.5	-7.8	-12	5	1	18.3	-19.8	-13	2	2•	2.5	1.7	-14	2	2•	2.1	-2.1
10	-11	0	12.0	-12.7	-11	4	1•	3.7	-.7	11	-11	0	5.3	5.3	12	5	-2	7.9	-9.4	13	2	-3•	2.4	2.3	14	2	-3	5.6	-6.9
10	-11	1	4.1	-4.1	11	4	2	2.9	-.8	11	-11	1•	2.1	.3	-12	5	2	16.4	-16.4	-13	2	3•	2.8	3.4	-14	2	3	12.4	14.3
-10	11	1	9.0	-9.2	11	-4	2	4.5	1.5	-11	11	1•	3.1	6.1	12	5	-3•	2.3	.0	13	2	-4•	2.8	1.2	14	2	-4	4.7	-5.0
-10	11	2	7.5	-7.6	-11	4	2•	3.0	-1.8	-11	11	2•	2.6	-1.5	-12	5	3•	2.7	-2.1	-13	2	4•	3.0	-2.7	-14	2	4	10.4	10.5
-10	11	3	8.2	-8.7	11	4	-3•	2.7	-2.1	-11	11	3•	2.4	-.8	12	5	-4	10.4	-12.6	13	2	-5	8.8	8.8	14	2	-5	9.8	-11.9
-10	11	4	6.7	-6.9	-11	4	3•	2.9	1.7	-11	11	4•	2.3	2.0	-12	5	4	7.8	-8.0	-13	2	5•	2.9	-1.5	-14	2	5•	2.6	2.1
-10	11	5•	2.0	.0	11	4	-4•	3.1	4.0	-11	11	5•	1.6	-2.6	12	5	-5•	2.3	-2.4	13	-3	0•	3.6	1.1	-14	3	2	3.1	3.0
10	-12	0	8.8	-7.8	-11	4	4•	3.0	-.8	11	-12	0•	3.1	1.3	-12	5	5•	3.0	1.2	13	3	-1•	1.9	-2.1	-14	3	3	11.7	13.3
10	-12	1	10.0	-9.7	11	4	-5	8.9	9.3	-11	12	1•	2.8	4.1	12	-6	0•	4.2	-4.3	-13	3	1•	3.0	-.1	-14	3	4	7.6	6.7
-10	12	1	7.4	-7.1	-11	4	5	7.8	6.7	-11	12	2	6.4	-7.2	12	6	-1•	.8	-2.4	13	3	-2	3.3	2.9	-14	3	5	5.8	4.4
-10	12	2•	2.6	-2.6	11	5	0•	3.4	-3.3	-11	12	3•	2.0	-.3	12	-6	1	15.5	-15.2	-13	3	2•	3.0	1.5	-14	4	2•	2.4	3.9
-10	12	3	7.0	7.8	11	-5	0•	4.6	-4.5	-11	12	4•	2.0	7.3	-12	6	1	11.4	-12.0	13	3	-3•	2.3	-.9	-14	4	3	4.6	5.9
-10	12	4•	2.6	1.2	11	5	-1•	3.3	-2.3	12	0	0	14.2	14.3	12	6	-2	7.5	-8.7	-13	3	3•	2.8	.8	-14	4	4•	3.0	.4
10	-13	0•	3.4	3.5	11	-5	1•	3.5	-1.9	12	0	1	11.3	11.5	-12	6	2•	2.9	-2.5	13	3	-4•	2.4	.4	-14	4	5	5.1	-4.5
-10	13	1•	2.8	-5.6	-11	5	1•	3.8	-2.8	12	0	-1	8.8	8.8	12	6	-3•	2.1	1.0	-13	3	4•	3.0	-1.4	-14	5	1•	2.3	1.5
-10	13	2•	2.3	2.9	11	5	-2	6.6	7.9	12	0	-2	9.9	10.8	-12	6	3•	2.4	2.4	13	3	-5	7.8	8.6	-14	5	2•	2.4	-3.7
-10	13	3	11.7	13.4	11	-5	2•	2.9	-3.0	12	0	-3	13.0	13.7	12	6	-4	9.4	-10.7	-13	3	5	5.6	-4.4	-14	5	3•	2.3	-.4
-10	14	1•	1.8	5.0	-11	5	2•	3.0	.9	12	0	-4•	3.0	.6	-12	6	4	11.6	11.6	-13	4	1•	3.2	2.9	-14	5	4	7.2	-7.4
11	0	0•	4.5	-.2	11	5	-3	4.0	-4.0	12	0	-5	5.3	-4.3	12	6	-5	8.4	-9.3	13	4	-2•	1.8	1.4	-14	5	5	12.4	-13.7
11	0	1•	3.2	3.5	-11	5	3	8.9	8.1	12	1	0	8.8	9.0	-12	6	5	7.0	6.6	-13	4	2•	2.7	-2.8	-14	6	2	9.9	-11.0
11	0	-1•	3.7	1.2	11	5	-4•	3.0	-.0	12	-1	0	13.1	14.5	12	-7	0•	4.1	4.8	13	4	-3•	2.1	-.7	-14	6	3	6.6	-7.4
11	0	-2•	3.0	-1.1	-11	5	4	8.7	7.6	12	1	-1•	3.5	3.4	12	-7	1	14.5	-5.9	-13	4	3•	2.6	-1.3	-14	6	4	9.6	-10.0
11	0	-3	4.8	-5.4	11	5	-5	7.5	8.3	12	-1	1	8.2	8.8	-12	7	1•	3.2	-.9	13	4	-4	4.8	-5.2	-14	6	5	10.9	-12.9
11	0	-4•	3.0	-1.4	-11	5	5•	3.0	2.0	-12	1	1•	3.4	3.3	12	7	-2•	.8	-4.1	-13	4	4•	3.0	-3.1	-14	7	2	13.2	-15.3
11	0	-5•	3.1	-1.4	11	6	0•	2.7	-1.8	12	1	-2	16.9	18.5	-12	7	2	9.3	8.9	13	4	-5	3.6	3.7	-14	7	3	8.3	-9.0
11	1	0•	4.6	-5.5	11	-6	0	6.7	-6.5	-12	1	2•	2.9	-.7	12	7	-3•	1.7	-1.9	-13	4	5	3.7	-3.4	-14	7	4	3.5	-2.4
11	-1	0•	4.6	1.9	11	6	-1•	2.7	1.0	12	1	-3	11.2	11.5	-12	7	3	14.2	14.6	13	-5	0•	3.5	4.3	0	0	0a	-.0	-3.6
11	1	1	3.1	2.2	11	-6	1	6.3	-7.1	-12	1	3	16.9	17.7	12	7	-4	4.3	-6.2	-13	5	1•	3.1	2.5	0	0	0a	.0	.0
11	1	-1•	3.8	-.4	-11	6	1•	3.8	.7	12	1	-4	10.9	10.0	-12	7	4	11.6	12.5	13	5	-2•	1.0	.2	0	0	0a	.0	.0
11	-1	1•	3.3	5.0	11	6	-2	4.1	4.1	-12	1	4	13.1	-12.0	-12	7	5	4.9	5.7	-13	5	2•	2.9	-.9	0	0	0a	.0	.0

TABLE II.

Final atomic parameters and their standard deviations (in parentheses).

The letter *w* labels the oxygen atoms belonging to water molecules. B is the equivalent isotropic temperature factor after Hamilton (8).

ATOMS	x/a	y/b	z/c	B(Å^2)
Na(1) . . .	0.0748 (2)	0.9749 (2)	0.3343 (4)	3.70
Na(2) . . .	0.4132 (2)	0.9923 (2)	0.6610 (4)	3.31
S(1)	0.1729 (2)	0.1085 (1)	0.0662 (3)	2.57
S(2)	0.2000 (2)	0.3108 (1)	0.3691 (3)	4.84
S(3)	0.3313 (2)	0.8851 (1)	0.9648 (3)	2.68
S(4)	0.3445 (3)	0.6729 (2)	0.1308 (4)	7.05
O(1)	0.1034 (5)	0.2796 (4)	0.9314 (8)	4.64
O(2)	0.3452 (6)	0.7143 (4)	0.7563 (9)	6.14
O(3)*w* . . .	0.4667 (4)	0.1163 (4)	0.4455 (8)	3.68
O(4)*w* . . .	0.0336 (4)	0.8851 (4)	0.5984 (8)	3.67
O(5)*w* . . .	0.2255 (5)	0.8700 (4)	0.3430 (9)	4.60
O(6)*w* . . .	0.2633 (5)	0.1035 (4)	0.6577 (8)	3.93
C(1)	0.1583 (6)	0.2390 (5)	0.1190 (12)	3.11
C(2)	0.0772 (12)	0.3905 (7)	0.9439 (18)	8.61
C(3)	0.0148 (11)	0.4094 (8)	0.7095 (17)	7.85
C(4)	0.3427 (7)	0.7511 (5)	0.9456 (12)	3.42
C(5)	0.3614 (11)	0.6026 (7)	0.7084 (19)	7.94
C(6)	0.5021 (13)	0.6062 (9)	0.7908 (29)	12.80

TABLE III.

Final anisotropic thermal parameters ($\times 10^4$) *and their standard deviations (in parentheses).*

The anisotropic temperature factors are in the form:

$$\exp\left[-\left(h^2 \beta_{11} + k^2 \beta_{22} + l^2 \beta_{33} + 2\, hk\, \beta_{12} + 2\, hl\, \beta_{13} + 2\, kl\, \beta_{23}\right)\right]$$

ATOM	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Na(1) . .	55 (3)	81 (2)	230 (9)	30 (2)	52 (4)	24 (3)
Na(2) . .	54 (3)	66 (2)	222 (9)	20 (1)	58 (4)	24 (3)
S(1) . .	63 (2)	41 (1)	157 (5)	20 (1)	44 (2)	16 (2)
S(2) . .	166 (3)	44 (1)	246 (7)	9 (2)	112 (4)	—7 (2)
S(3) . .	60 (2)	41 (1)	170 (5)	20 (1)	39 (2)	25 (2)
S(4) . .	276 (5)	43 (1)	393 (9)	38 (2)	214 (6)	57 (3)
O(1) . .	144 (7)	47 (3)	262 (18)	38 (4)	74 (8)	37 (6)
O(2) . .	197 (9)	63 (4)	363 (23)	27 (5)	176 (12)	1 (7)
O(3) . .	61 (5)	70 (4)	253 (16)	27 (4)	59 (7)	35 (6)
O(4) . .	54 (5)	65 (4)	279 (17)	16 (3)	55 (7)	24 (6)
O(5) . .	83 (6)	70 (4)	366 (20)	21 (4)	104 (9)	5 (7)
O(6) . .	90 (5)	70 (4)	237 (17)	37 (4)	90 (8)	37 (6)
C(1) . .	72 (7)	37 (4)	274 (25)	8 (4)	72 (11)	18 (8)
C(2) . .	308 (21)	54 (6)	529 (42)	91 (10)	181 (24)	68 (13)
C(3) . .	232 (17)	92 (8)	500 (42)	95 (10)	177 (22)	110 (14)
C(4) . .	86 (8)	41 (4)	240 (25)	7 (5)	81 (11)	22 (8)
C(5) . .	233 (17)	64 (7)	626 (47)	45 (9)	259 (24)	3 (14)
C(6) . .	210 (19)	95 (10)	1552 (105)	93 (11)	383 (39)	184 (26)

TABLE IV.

Analysis of the anisotropic thermal parameters.

(root mean square thermal vibrations along the ellipsoid axes (Å), magnitudes of the principal axes (Å^2) and angles (°) between the crystallographic axes and the principal axes of the vibration ellipsoids).

ATOM	*r.m.s.*	B	α	β	γ
Na(1) . . .	0.20	3.26	100	85	20
	0.25	4.88	80	20	105
	0.15	1.86	15	110	102
Na(2) . . .	0.19	3.10	92	93	24
	0.22	3.86	87	14	99
	0.16	1.93	3	103	113
S(1)	0.17	2.20	89	96	26
	0.19	2.88	42	58	112
	0.16	2.00	132	32	77
S(2)	0.21	3.65	110	128	33
	0.30	7.23	23	106	92
	0.16	2.08	101	43	57
S(3)	0.18	2.56	101	60	41
	0.19	2.83	34	67	124
	0.15	1.83	122	40	110
S(4)	0.23	4.16	116	76	20
	0.38	11.48	26	96	90
	0.16	2.08	88	16	110
O(1)	0.22	3.74	95	78	30
	0.29	6.51	16	84	116
	0.17	2.21	106	14	104
O(2)	0.25	4.82	66	44	135
	0.33	8.41	37	103	79
	0.18	2.62	116	48	47
O(3)	0.21	3.53	107	106	12
	0.23	4.18	84	28	83
	0.16	2.13	18	112	100
O(4)	0.22	3.81	98	21	79
	0.23	4.09	104	109	15
	0.16	2.15	16	98	100
O(5)	0.22	3.92	72	44	79
	0.27	5.76	87	124	35
	0.18	2.52	18	114	123
O(6)	0.20	3.22	103	50	133
	0.24	4.59	63	49	85
	0.17	2.24	150	67	44
C(1)	0.19	2.91	18	117	117
	0.22	3.89	86	101	29
	0.16	2.11	72	30	100

TABLE IV (*continued*).

ATOM	*r.m.s.*	B	α	β	γ
C(2)	0.30	7.20	100	90	17
	0.41	13.37	21	82	107
	0.14	1.66	108	8	93
C(3)	0.29	6.57	122	82	15
	0.36	10.39	41	70	91
	0.20	2.88	113	21	105
C(4)	0.19	2.96	124	62	34
	0.22	3.91	44	111	71
	0.17	2.18	65	36	117
C(5)	0.29	6.50	133	120	43
	0.37	10.92	56	102	59
	0.18	2.47	119	33	63
C(6)	0.30	6.88	38	62	116
	0.52	21.84	93	87	26
	0.19	2.98	128	28	87

TABLE V.

Atomic distances (Å), bond angles and their standard deviations (in parentheses).

Atomic distances	
S(1)—C(1)	1.698 (6)
S(2)—C(1)	1.650 (7)
C(1)—O(1)	1.336 (8)
O(1)—C(2)	1.480 (13)
C(2)—C(3)	1.480 (15)
S(1)—O(1)	2.535 (6)
S(1)—S(2)	2.983 (2)
S(2)—O(1)	2.608 (6)
S(3)—C(4)	1.710 (6)
S(4)—C(4)	1.642 (8)
C(4)—O(2)	1.321 (11)
O(2)—C(5)	1.474 (11)
C(5)—C(6)	1.474 (19)
S(3)—O(2)	2.521 (6)
S(3)—S(4)	2.980 (2)
S(4)—O(2)	2.604 (6)
Na(1)—S(1)	2.983 (3)
Na(1)—S(1′)	2.889 (3)
Na(1)—O(4)	2.343 (6)
Na(1)—O(4′)	2.450 (6)
Na(1)—O(5)	2.355 (6)
Na(1)—O(6)	2.474 (5)

Atomic distances	
Na(2)—S(3)	2.915 (3)
Na(2)—S(3′)	2.954 (3)
Na(2)—O(3)	2.386 (6)
Na(2)—O(3′)	2.381 (6)
Na(2)—O(5)	2.422 (5)
Na(2)—O(6)	2.411 (6)

Bond angles	
S(1)—C(1)—O(1)	112° 43′ (34′)
S(1)—C(1)—S(2)	125° 59′ (26′)
S(2)—C(1)—O(1)	121° 16′ (34′)
C(1)—O(1)—C(2)	120° 19′ (38′)
O(1)—C(2)—C(3)	106° 43′ (47′)
S(3)—C(4)—O(2)	111° 55′ (33′)
S(3)—C(4)—S(4)	125° 29′ (32′)
S(4)—C(4)—O(2)	122° 33′ (32′)
C(4)—O(2)—C(5)	121° 28′ (44′)
O(2)—C(5)—C(6)	110° 2′ (53′)

TABLE VI.

Hydrogen atoms parameters from difference Fourier synthesis.

ATOMS	x/a	y/b	z/c
H(1)	0.523	0.179	0.573
H(2)	0.376	0.114	0.328
H(3)	0.875	0.115	0.289
H(4)	0.035	0.173	0.392
H(5)	0.766	0.191	0.566
H(6)	0.742	0.125	0.773
H(7)	0.245	0.165	0.552
H(8)	0.235	0.105	0.781
H(9)	0.005	0.620	0.010
H(10)	0.175	0.440	0.070
H(11)	0.023	0.520	0.320
H(12)	0.115	0.415	0.730
H(13)	0.040	0.633	0.460
H(14)	0.304	0.542	0.750
H(15)	0.361	0.580	0.550
H(16)	0.430	0.400	0.030
H(17)	0.570	0.360	0.170
H(18)	0.448	0.345	0.280

TABLE VII.

Hydrogen atoms interatomic distances (Å) and angles.

ATOMS	BOND LENGTHS	ATOMS	BOND ANGLES
H(1)—O(3)	1.0	H(1)—O(3)—H(2)	124°
H(2)—O(3)	1.0		
H(3)—O(4)	1.0	H(3)—O(4)—H(4)	112°
H(4)—O(4)	1.0		
H(5)—O(5)	1.1	H(5)—O(5)—H(6)	111°
H(6)—O(5)	1.1		
H(7)—O(6)	1.1	H(7)—O(6)—H(8)	118°
H(8)—O(6)	1.0		
H(9)—C(2)	1.1	H(9)—C(2)—H(10)	118°
H(10)—C(2)	1.1		
H(11)—C(3)	1.1	H(11)—C(3)—H(12)	117°
H(12)—C(3)	1.1	H(11)—C(3)—H(13)	95°
H(13)—C(3)	1.1	H(12)—C(3)—H(13)	100°
H(14)—C(5)	1.1	H(14)—C(5)—H(15)	114°
H(15)—C(5)	1.1		
H(16)—C(6)	1.1	H(16)—C(6)—H(17)	97°
H(17)—C(6)	1.1	H(16)—C(6)—H(18)	111°
H(18)—C(6)	1.0	H(17)—C(6)—H(18)	116°

DESCRIPTION AND DISCUSSION OF THE CRYSTAL STRUCTURE.

The crystal structure of sodium xanthate dihydrate (fig. 1) is marked by the presence of NaS_2O_4 octahedra conjunct in layers parallel to (010) and of xanthate groups lying between such layers.

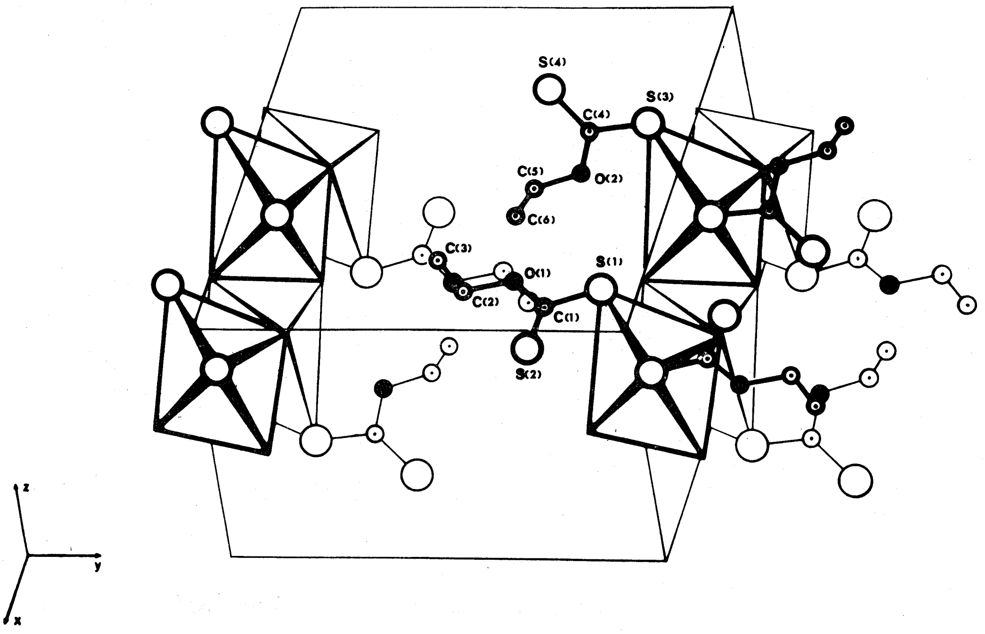


Fig. 1. – Clinographic projection of the unit cell of sodium xanthate dihydrate.

The corners of the two non-equivalent octahedra around sodium atoms are occupied by two sulfur atoms belonging to different xanthate groups and four oxygens of water molecules. The octahedra are fairly distorted as a consequence both of the different bond lengths (Table V) occurring between Na–O (average value 2.40 Å) and respectively Na–S (average length 2.93 Å) and of the positions in the octahedra of the sulfur atoms, which are disposed at the extremities of an edge.

Each sodium octahedron (fig. 2) shares three of its edges with an equal number of similar octahedra (one of them crystallographically equivalent to it); in this way a layer is formed, with the octahedra connected in a sort of six-membered ring.

As each anion (sulfur or oxygen) is shared by two octahedra, the layer may be considered as built up on the repetition of the unit $NaSO_2$, comparable with that of the mineral gibbsite $Al(OH)_3$ and, actually, the layers of octahedra in the latter crystal structure are analogous to those in sodium xanthate, both deriving by a close packing of anions.

The octahedral layers are parallel to (010) and, in each layer, atoms of the same nature but crystallographically non–equivalent are located at distances of nearly one half of the *a*–period: in this way the presence of the cited pseudo–cell is clearly explained.

Pairs of xanthate groups, symmetrical for an inversion center, roughly aligned along *b*, lie between two layers of octahedra, which repeat themselves after an entire *b*–period.

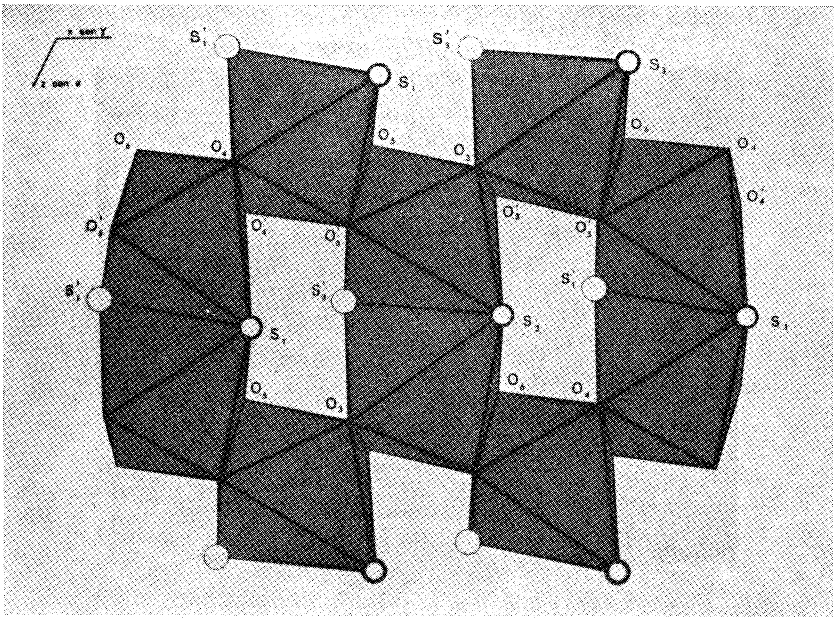


Fig. 2. – Projection along [010] of the layer of Na–octahedra in sodium xanthate dihydrate. The rings of six octahedra are shown.

Two non–equivalent xanthate radicals are in the unit cell, but in any case only one of their sulfur atoms takes part to the octahedral coordination around sodium atoms, whereas the remaining one is bound merely to the carbon atom of the xanthate molecule. The connection between octahedral layers and xanthate radicals is therefore practically obtained through one sulfur atom, apart from possible weak hydrogen bonds between the remaining sulfur atom and water molecules (fig. 3: distances ranging from 3.51 to 3.33 Å).

The oxygen atoms, as well as the remaining atoms of each xanthate group have simple intramolecular contacts with atoms of adjacent xanthate radicals. The most significative distances between atoms of different molecules are reported in fig. 3 : the shortest one is 3.24 Å. The presence of layers of Na–octahedra parallel to (010) and no strong bond between the same layers explain the perfect {010} cleavage.

The bond lengths between homologous atoms in the two non-equivalent xanthate groups are quite comparable. It appears noteworthy that the distance between carbon and the sulfur [S(1) or S(3)] joined to sodium atoms is in both cases larger than the distance between the same carbon and the ' free ' sulfur [S(2) or S(4)] (1.70–1.71 against 1.64–1.65 Å). Both distances are intermediate between the corresponding distances in thiols (1.80 Å) and carbon disulfide (1.55 Å). Furthermore the bonds C(1)–O(1) and C(4)–O(2) are sensibly shorter (1.33 and 1.32 Å respectively) than those found in alcohols (1.42 Å) but too large for a double bond (1.21 Å). These considerations suggest the conclusion that in the xanthate molecules some resonance must take place among the following configurations:

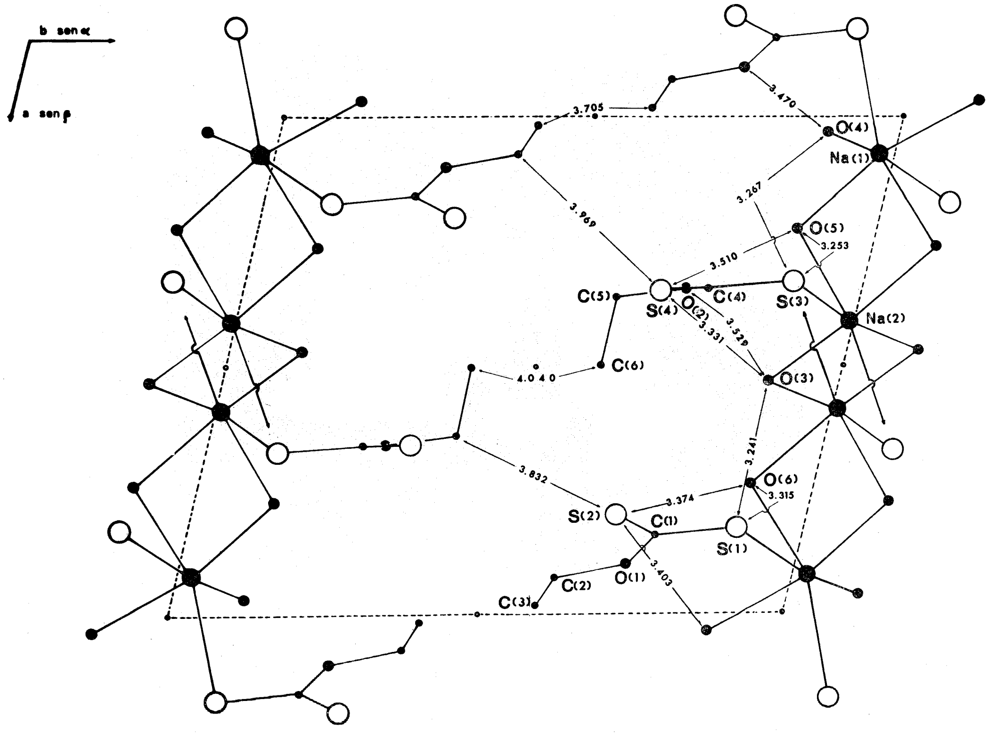
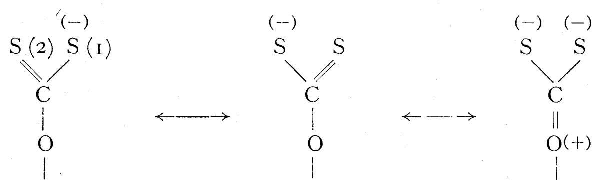


Fig. 3. – Representation of the disposition of the atoms in the unit cell of sodium xanthate dihydrate. The most significative intermolecular atomic distances are reported.



with a prevalence of the first of them as a consequence of the fact that S(2) [S(4) for the other non equivalent xanthate molecule] is not bound to sodium atoms.

The remaining O–C distances are not sensibly different from the values given by Sutton (4) for the alcohols (1.43 against 1.47–1.48 Å reported here). The distances C–C in the ethyl radical are instead rather short (1.48 against 1,54 Å, average value for olefins given by Sutton), but this contraction is probably only apparent, due to the considerable thermal motion (Table IV) of C(2), C(3), C(5) and C(6); anyway, in different xanthates or analogous compounds, particularly short distances between carbons of ethyl groups were already found [1.49 Å, Gottardi [5] – 1.50 Å, Ikeda [6] – 1.47 Å, Parthasarathy [7]].

No relevant particularity is shown by the bond angles in the xanthate molecules (Table V): the obtained values agree with those found in different xanthates.

Whereas both non–equivalent xanthate radicals are quite similar as far as bond lengths and angles are concerned, a noteworthy difference is given by the fact that only one of the two molecules [that of S(1), S(2), ...] is, in the limit of the standard deviations of atomic parameters, completely planar. In the second xanthate molecule, all the atoms lie in a plane with the exception of C(6), which reaches the maximum distance from the same plane allowed by the C–C bond, and forms with the plane itself an angle of 70° 24′: the removal of C(6) from the plane of the remaining atoms is very likely due to sterical hindrance between the same carbon atom and sulfur S(2) of an adjacent xanthate radical.

The plane of the xanthate molecule S(1), S(2), ... is nearly perpendicular to (001): the angle between these planes is in fact 85° 30′. The plane of all the atoms, but C(6), of the second xanthate radical forms an angle of 61° 2′ with (001). The angle between the planes of the two non–equivalent xanthate groups is 25° 38′.

An interesting feature of the structure is also given by the high thermal vibration of the atoms of the xanthate radicals; such thermal motion increases the farther the atoms are from the sulfur joined to sodium atoms and it reaches extreme values for the last C–atoms in the xanthate chains. Very likely this feature is due to the fact that the only strong intermolecular bond in each xanthate radical is that between one of the sulfur atoms and sodium atoms.

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